2016 Graphene & Related Materials Conference (GRM-2016)

Bilkent University, Ankara, Turkey

July 13-15, 2016

Online Book of Abstracts

2016 Graphene & Related Materials Conference (GRM-2016) Activity Program

Time	**July 13 (Wednesday)**	**Time**	**July 14 (Thursday)**	**Time**	**July 15 (Friday)**
9:00-9:20	**Opening Remarks**	9:00-9:40	**Francios Peeters (Invited Talk)** *Atomic collapse in graphene*	9:00-9:40	**Ekmel Özbay (Invited Talk)** *Graphene Based Tunable Photonic Metamaterials*
9:20-10:00	**Guy Le Lay (Invited Talk)** *Silicene, from Stripes to Sheets*	9:40-10:00	**Gözde Özbal** *A Mechanical Chain Reaction on Graphene at a Substrate Edge*	9:40-10:00	**Vahid Sazgari** *Large conductance fluctuation and localization in suspended monolayer graphene*
10:00-10:20	**Yasemin Çelik** *Effect of heating atmosphere on graphene growth during low pressure CVD*	10:00-10:20	**Mehmet Emin Kılıç** *Adsorption and diffusion on new two dimensional carbon allotropes (graphyne)*	10:00-10:20	**Eren Güvenilir** *Theoretical Investigation of Conductance and Quantum Capacitance of Quantum Hall Effect Edge states*
10:20-10:40	**Umut Kamber** *Formation of Fractal Structures at the Graphene-Copper Interface During Chemical Vapor Deposition*	10:20-10:40	**Deniz Keçik** *Tunable Optoelectronic Properties of Graphene by Charge Doping*	10:20-10:40	**Hakan U. Özdemir** *Electronic and Spintronic Properties of Disordered Zigzag Graphene Nanoribbons*
10:40-11:00	**Break**	10:40-11:00	**Break**	10:40-11:00	**Break**
11:00-11:20	**Seymur Cahangirov** *Atomic and electronic properties of SnS2 and WTe* 2	11:00-11:20	**Timur Ashirov** *A Facile Method for Clean Graphene Transfer Based on Sacrificial Photoresist Layer*	11:00-11:20	**Doolos Aibek Uulu** *Controlled Perforation of Freestanding Graphene by Focused Ion and Electron Beams*
11:20-11:40	**Mehmet Yağmurcukardeş** *Ultra-Ductile Monolayers of GaS and GaSe*	11:20-11:40	**Arda Balkancı** *The Influence of Interface Size and Topography on the Nanotribology of Graphene*	11:20-11:40	**Khaydarali Sayfidinov** *Large Area Monolayer Graphene Oxide Synthesis by Controlled Oxidation*
11:40-12:00	**Selma Şenozan** *Restacking effects on the electronic properties of bilayer 1T phase of MoS2*	11:40-12:00	**Ceren Sibel Sayın** *Friction of Graphene over 4H-SiC{0001} Surfaces*	11:40-12:00	**Ali Haider** *Structural and Optical Properties of h-BN Thin Films Deposited by Sequential Exposures of Triethylboron and N2/H2 Plasma*
12:00-12:20	**Cem Sevik** *Peculiar Piezoelectric Properties of Two-Dimensional Materials*	12:00-12:40	**Coşkun Kocabaş (Invited Talk)**	12:00-12:20	**Closing Remarks**
12:20-12:40	**Engin Durgun** *GaN: From three- to two-dimensional single-layer crystal and its multilayer van der Waals solids*	12:40-14:30	**Lunch and Poster Session**		
12:40-14:30	**Lunch and Poster Session**	14:30-15:10	**Klaus Ensslin (Invited Talk)** *Graphene Quantum Devices*		
14:30-15:10	**Şefik Süzer (Invited Talk)** *Chemical and Electrical Characterization of Graphene-Based Devices with XPS*	15:10-15:30	**Mert Taşkın** *Atomic and Island Scale Diffusion Events on Bi2Te3 (0001) Surface*		
15:10-15:30	**Uğur Y. İnkaya** *Graphene-based flexible Hall sensor*	15:30-15:50	**H. Tunç Çiftçi** *Photon Emission from Graphene/Copper Interface in a Tunnel Junction*		
15:30-15:50	**İsmet İ. Kaya** *Multilayer Graphene Based Passive Matrix OLED Displays*	15:50-16:10	**Cem Kıncal** *Swift Heavy Ion Irradiation of Graphene Layers on HOPG*		
15:50-16:10	**Cem Çelebi** *Epitaxial Graphene Contact Electrode for Optoelectronics Device Applications*	16:10-16:30	**Nasima Afsharimani** *Comparative STM Study of Self-Assembled Alkanethiol Monolayers on HOPG and Single-Layer Graphene*		

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Oral Presentations

July 13, Wednesday

Silicene, from Stripes to Sheets

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According to a recent Thomson-Reuters citation-based study of the 10 hottest research fronts identified in physics, “Silicene growth and properties”, just next to “Observation of Higgs boson”, “Globalneutrino data analysis” and “Nonlinear massive gravity”, is first in condensed matter physics [1]. Silicene *sheets* were first synthesized in 2012 on a silver (111) substrate in the form of the archetype $3\times3/4\times4$ phase [2]. This artificial two-dimensional (2D) honeycomb allotrope of silicon appears as a promising candidate for ultimate scaling of nanoelectronic devices [3]. Multi-layer silicene, which hosts Dirac fermions and which is stable in ambient air, protected by its ultra-thin native oxide, was formed next [4,5], as well as single and multilayer germanene [6,7] and monolayer stanene [8,9]. Yet, the advent of silicene *sheets* on Ag(111) was preceded by the growth of massively parallel one-dimensional atom-thin silicon *stripes* on Ag(110). The strongly debated nature of these *stripes* has just been elucidated and proved to be penta-silicene nano-ribbons composed only of pentagonal Si building-blocks [10].

In this invited talk, I will describe all these findings and discuss the tantalizing prospects offered by these artificial low dimensional elemental allotropes beyond graphene.

[1] C. Day, Physics Today, 25 September 2015.

[2] P. Vogt *et al.*, Phys. Rev. Lett., **108**, 155501 (2012).

[3] Tao *et al.*, Nature Nanotechnol., 10, 227 (2015)

[4] P. De Padova *et al.*, 2D Mater., **1**, 021003 (2014).

[5] G. Le Lay, E. Salomon and T. Angot, Europhysics News, **47**, 17 (2016).

[6] M. E. Dávila, L. Xian, S. Cahangirov, A. Rubio and G. Le Lay, New Journal of Physics, **16**, 095002 (2014).

[7] M. E. Dávila and G. Le Lay, Sci. Rep., **6**, 20714 (2016).

[8] Feng-feng Zhu *et al.*, Nature Materials, **14**, 1020 (2015).

[9] J. Yuhara *et al.*, to be published.

[10] J. I. Cerdá *et al.*, arxiv.org:443/find/all/1/OR+au:penta_silicene+all:+EXACT+penta_silicene/0/1/0/all/0/1

2016 Graphene & Related Materials Conference (GRM-2016), Ankara, Turkey
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Effect of heating atmosphere on graphene growth during low pressure chemical vapor deposition

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[2] Université Toulouse III Paul Sabatier, INP, Institut Carnot Cirimat, 118 Route de Narbonne, F-31062 cedex 9 Toulouse, France
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Low-pressure chemical vapor deposition (CVD) synthesis of graphene films on Cu foil was performed by controlling H_2 and/or Ar flow rates during heating. The heating atmosphere affected not only nucleation of graphene, but also type and amount of impurities formed on the surface. H_2 and Ar/H_2 heating resulted in the formation of spherical nanometer-sized impurities, while irregular-shaped, large (a few μm) SiO_2 impurities were observed when Ar alone was used during heating. The formation of these large SiO_2 particles was attributed to oxidation of Si impurities already present in the Cu foil before the CVD process. The effect of difference in Cu foil characteristics on graphene growth, i.e., surface oxygen content, was also examined. In case of using oxygen-free Cu foil, heating in H_2 flow resulted in deactivation of the foil surface by surface bound hydrogen atoms, while graphene growth (accompanied with the formation of large SiO_2 particles) was promoted when Ar flow only was used. On oxygen-rich Cu foil, Ar heating resulted in a much higher amount of SiO_2 impurities, while presence of H_2 in the heating atmosphere promoted high quality graphene growth without large SiO_2 impurities. Quantum Hall Effect measurements confirmed that the grown material was monolayer graphene.

Please indicate your preference:

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Formation of Fractal Structures at the Graphene-Copper Interface During Chemical Vapor Deposition

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[2]Koç University, Chemistry Department, Rumeli Feneri Yolu, 34450, Sarıyer, İstanbul, Turkey

Chemical Vapor Deposition (CVD) is an efficient method for producing large area graphene on metal foils. Improving the graphene quality is one of the most intensely worked subtopic in graphene research, yet there are still apparent factors affecting the quality of the CVD-grown graphene. It has been known since the first CVD growth of graphene on Cu foils in a quartz tube that some droplet like silicon-oxide contaminants appear on the surfaces [1]. Recently it has been shown that these contaminants occur before the growth of graphene and they are quite mobile on the copper surface [2]. We have performed CVD processes with different parameters in order to control the shapes and sizes of these silicon-oxide contaminants. We discovered the formation of silicon-oxide fractal structures and developed the methodology to generate different shapes and sizes of nano scale dendritic structures during graphene growth by AP-CVD on Cu foils. We also investigated the formation of similar structures on bare Cu foils. Here, we will present a novel method to produce silicon-oxide dendritic nano particles with uniform distribution on Cu foils [3].

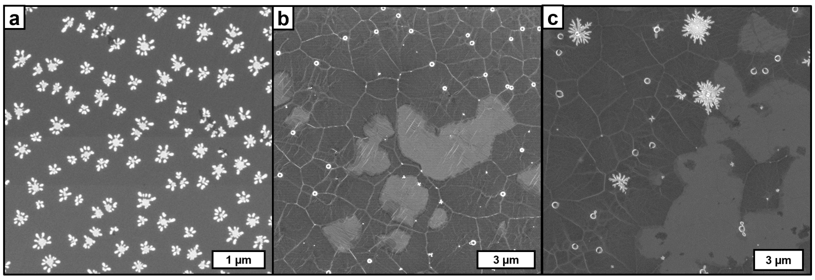

Figure: Scanning Electron Micrographs of (a) silicon-oxide particles on bare copper surface, (b) point-like impurities at the graphene/copper interface and (c) silicon-oxide fractals on graphene/copper surface.

This work was supported by TÜBİTAK-1003 project with grant number 114F036.

[1] X. Li et al., Science 324, 1312 (2009).

[2] Z.J. Wang et al., ACS Nano 9, 2, 1506-1519 (2015).

[3] U. Kamber et al, *Formation of silicon-oxide fractals during chemical vapor deposition growth of graphene on copper foils.* (submitted) (2016).

Please indicate your preference:

Oral Presentation: [x]

Poster Presentation: []

Atomic and electronic properties of SnS$_2$ and WTe$_2$

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Synthesis of graphene boosted research on other 2D materials including silicene, germanene, group III-V honeycomb structures, transition metal dichalcogenides and others. We have recently studied the atomic and electronic structure of two newcomers of 2D family, SnS$_2$ and WTe$_2$. We show that the energy difference between different stacking configuration of SnS$_2$ is significantly smaller compared to transition metal dichalcogenides. It is possible to manipulate the stacking by applying perpendicular pressure or by charging the system. We also revealed the anisotropic electronic, mechanical and optical properties of WTe$_2$. We find that the Poisson ratio and the in-plane stiffness is direction dependent due to the symmetry breaking induced by the dimerization of the W atoms along one of the lattice directions of the compound. Since the semimetallic behavior of the Td phase originates from this W-W interaction, tensile strain along the dimer direction leads to a semimetal to semiconductor transition after 1% strain.

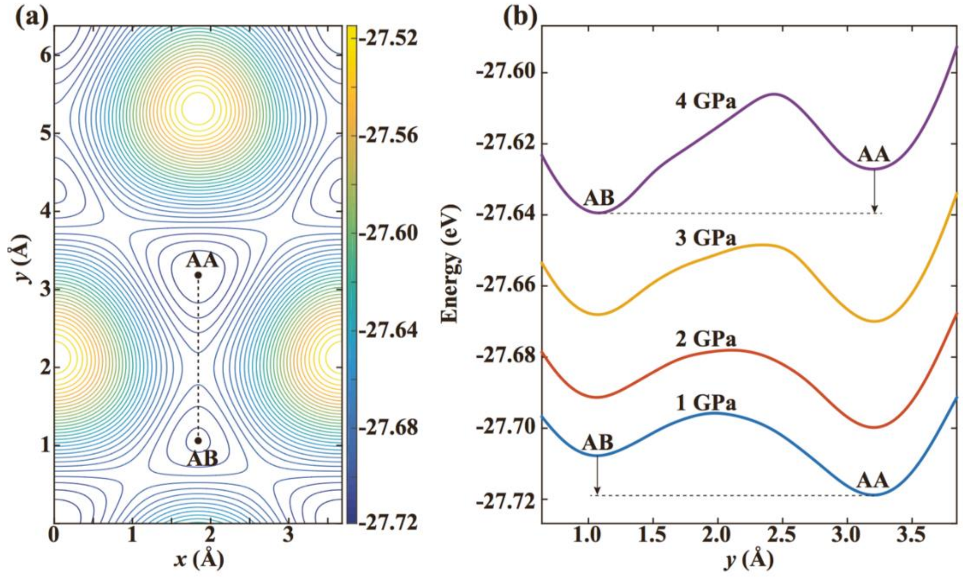

Figure 1: (a) Constant-height energy landscape of bilayer SnS2. (b) Constant-pressure energy dependence along the line connecting AA and AB stackings.

[1] C. Bacaksiz *et al.*, Physical Review B **93**, 125403 (2016).

[2] E. Torun *et al.*, Journal of Applied Physics **119**, 074307 (2016).

Please indicate your preference:

Oral Presentation: [x]

Ultra-Ductile Monolayers of GaS and GaSe

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The mechanical properties of monolayer GaS and GaSe crystals are investigated in terms of the in-plane stiffness (C), Poisson ratio (v), Young modulus (E), and ultimate strength (σ_U) by means of first-principles calculations. The calculated elastic parameters are compared with those of graphene and monolayer MoS_2. Our results indicate that due to the more ionic character of Ga-S bonds in comparison to the Ga-Se bonds, monolayer GaS is a stiffer material than monolayer GaSe crystals. In parallel to their in-plane stiffness, the effective Young modulus of GaS is also higher than that of monolayer GaSe. Although their Poisson ratio values are very close to each other, 0.26 and 0.25 for GaS and GaSe, respectively, monolayer GaS is a stronger material than GaSe monolayer due to its slightly higher σ_U value. For monolayer GaS and Gase crystals all these elastic parameters are smaller than those of graphene and monolayer MoS_2. However, GaS and GaSe crystals are found to be more ductile and flexible materials than graphene and MoS_2. We have also analyzed the band gap response of GaS and GaSe monolayers to biaxial tensile strain and predicted a semiconductor-metal crossover after 15\% and 13\% applied strain for monolayer GaS and GaSe, respectively. In addition, the effect of charging the system on the elastic constants are investigated. Our results demonstrate that adding charge to the system strongly decreases the values of C and E which makes the materials more flexible.

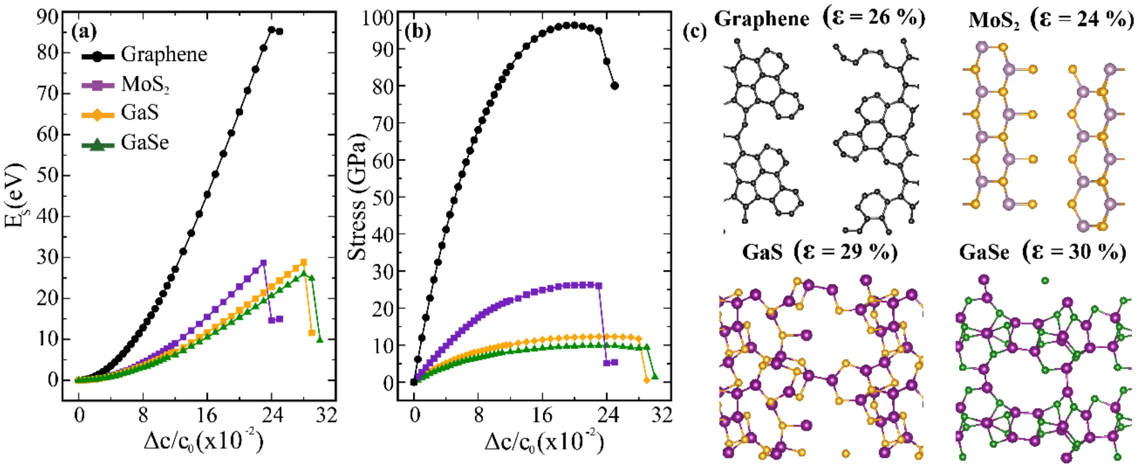

Figure: (a) The change of strain energy and (b) the created stress in the monolayer structure under applied biaxial strain. (c) The geometries of each monolayer crystals at fracture strain values.

This work is supported through the TUBITAK Project No. 114F397.

Please indicate your preference:

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Poster Presentation: [ ]

Restacking effects on the electronic properties of bilayer 1T phase of MoS2

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In this study, we have employed the density functional theory (DFT) to investigate the Van der Waals (vdW) interlayer spacing between the two layers of bilayer 1T phase of MoS2 (1T-MoS2) and the superstructures derived from bonding associations of metal atoms of restacked 1T-MoS2[1]. We observed that Mo atoms form clusters of Mo-Mo trimetrization on the two layers of bilayer system after geometric optimization. The vdW interlayer distance (equilibrium interlayer distance) has been optimized using DFT by computing the total energy as a function of the interlayer distance d, which was varied between 5Å and 7Å while keeping the in-plane lattice constant fixed at the bulk value. In order to evaluate the binding energy in 1T-MoS2 bilayer system energy difference has been evaluated between the total energy values at equilibrium distance and at d=7Å , which gives a value for the limit of infinite layer distance for 1T-MoS2. Recently experimental researches have focused on the exfoliation of layered materials to two dimensional nanosheets and then restacking them to form electrodes [2-6]. We observed that metallic 1T-MoS2 can intercalate ions efficiently which shows that 1T phase of MoS2 can be used as supercapacitor electrode materials.

[1] J. Am. Chem. Soc. 121, 638-643, 1999

[2] Nano Lett. 8, 3498-3502, 2008

[3] Science 341, 1502-1505, 2013

[4] Science 332, 1537-1541, 2011

[5] J. Am. Chem. Soc. 133, 17832-17838, 2011

[6] Nature Nanotechnology 10, 313-318, 2015

Please indicate your preference:

Oral Presentation: [X]

Peculiar Piezoelectric Properties of Two-Dimensional Materials

Deniz Çakır[1], Oguz Gulseren[2], Francois M. Peeters[1], Cem Sevik[3]
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[3]Department of Mechanical Engineering, AnadoluUniversity, Eskisęhir, TR 26555, Turkey

Recently, two dimensional materials with noncentrosymmetric structure have received significant interest due to their potential usage in piezoelectric applications. It has been reported by first principles calculations that relaxed-ion piezoelectric strain (d_{11}) and stress (e_{11}) coefficients of some transition metal dichalcogenide monolayers are comparable or even better than that of conventional bulk piezoelectric materials. Furthermore, piezoelectric coefficient of MoS_2 has been measured as 2.9×10^{-10} C/m, which agrees well with mentioned theoretical calculations [1]. In order to deeply investigate this potential, we perform first-principles calculations and systematically investigate the piezoelectric properties various single layer structures [2]: Two dimensional transition metal dichalcogenides (TMDCs), transition metal oxides, and II-VI compounds. We predict that not only the Mo- and W-based TMDCs but also the other materials with Cr, Ti, Zr and Sn exhibit highly promising piezoelectric properties. Moreover, we surprisingly observe that the calculated d_{11} coefficient of some II-VI compounds are quite larger than that of TMDCs and the bulk materials, α-quartz, w-GaN, and w-AlN which are widely used in current applications, see Figure 1. Our calculations clearly reveal that monolayer semiconductors are strong candidates for future atomically thin piezoelectric applications such as transducers, sensors, and energy harvesting devices.

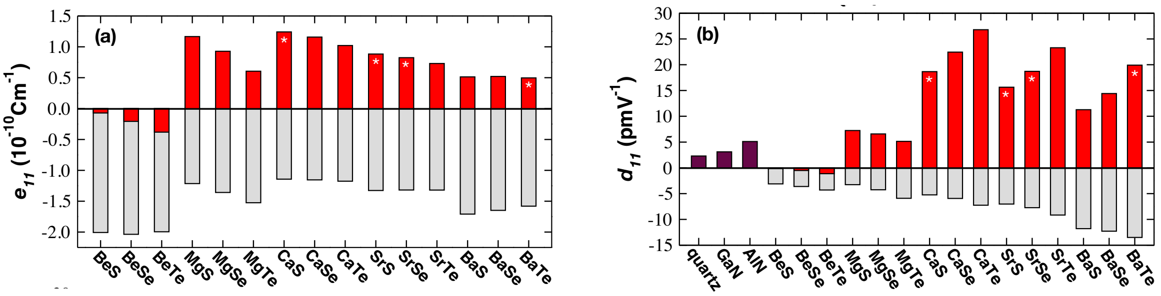

Figure 1: Calculated clamped- and relaxed-ion (a) piezoelectric stress (e_{11}) and (b) piezoelectric strain (d_{11}) coefficients for MX monolayers (where M= Be, Mg, Ca, Sr and Ba). Red (gray) bars depict the relaxed-ion (clamped-ion) piezoelectric coefficients. For comparison, d_{11} coefficient of α-quartz, GaN and AlN are also depicted in (b).

[1] H. Shu et al. Nat. Nano. 10, 151, 2014
[2] M. M. Alyoruk et al. J. Phys. Chem. C 119, 23231, 2015

Please indicate your preference:

Oral Presentation: [X]

Poster Presentation: [ ]

GaN: From three- to two-dimensional single-layer crystal and its multilayer van der Waals solids

A. Onen,[1,2] D. Kecik,[1] S. Ciraci[3] and E. Durgun[1,2]

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Three-dimensional (3D) GaN is a III-V compound semiconductor with potential optoelectronic applications. In this paper, starting from 3D GaN in wurtzite and zinc-blende structures, we investigated the mechanical, electronic, and optical properties of the 2D single-layer honeycomb structure of GaN (g−GaN) and its bilayer, trilayer, and multilayer van der Waals solids using density-functional theory. Based on high-temperature ab initio molecular-dynamics calculations, we first showed that g−GaN can remain stable at high temperature. Then we performed a comparative study to reveal how the physical properties vary with dimensionality.

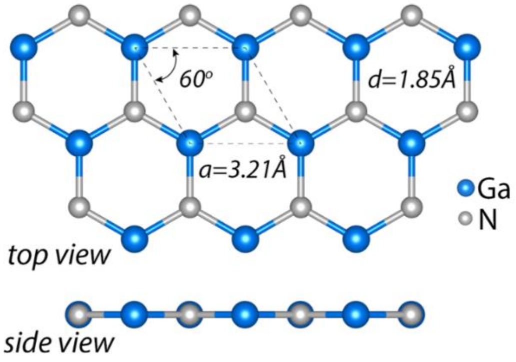

Figure: Top and side views of the optimized atomic structure of g-GaN.

While 3D GaN is a direct-band-gap semiconductor, g−GaN in two dimensions has a relatively wider indirect band gap. Moreover, 2D g−GaN displays a higher Poisson ratio and slightly less charge transfer from cation to anion. In two dimensions, the optical-absorption spectra of 3D crystalline phases are modified dramatically, and their absorption onset energy is blueshifted. We also showed that the physical properties predicted for freestanding g−GaN are preserved when g−GaN is grown on metallic as well as semiconducting substrates. In particular, 3D layered blue phosphorus, being nearly lattice-matched to g−GaN, is found to be an excellent substrate for growing g−GaN. Bilayer, trilayer, and van der Waals crystals can be constructed by a special stacking sequence of g−GaN, and they can display electronic and optical properties that can be controlled by the number of g−GaN layers. In particular, their fundamental band gap decreases and changes from indirect to direct with an increasing number of g−GaN layers [1].

[1]: A. Onen, D. Kecik, S. Ciraci and E. Durgun, Phys. Rev. B 93, 085431 (2016)

Oral Presentation: [X]

Chemical and Electrical Characterization of Graphene-Based Devices with XPS

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A noncontact chemical and electrical measurement technique of XPS is performed to investigate a number of devices under operation. The main objective of the technique is to trace chemical and location specified surface potential variations as shifts of the XPS peak positions under operating conditions. Devices consisting of graphene and other materials have been investigated by application of various external voltage bias, and under operating conditions. The main advantage of the technique is its ability to assess element-specific surface electrical potentials of devices under operation based on the energy deviation of core level peaks in surface domains/structures.

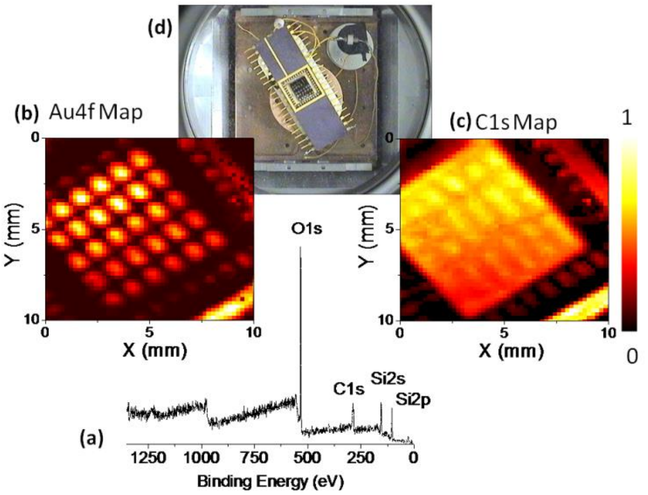

Figure: (a) A survey XP spectrum recorded from the graphene-only part. Areal intensity maps of the entire IC recorded in the snap-shot mode with 200 μm X-ray spot size and 200 μm steps of; (b) Au4f, and (c) C1s. (d) Picture of the IC inserted into the load-lock of the instrument.

[1] C. Kocabas and S. Suzer, *Analytical Chemistry* **85,** 4172 (2013).

[2] M. Copuroglu et al., *Nano Letters* **14**, 2837 (2014).

[3] P. Aydogan, O. Balci, C. Kocabas, S. Suzer, *Organic Electronics* (in press, 2016).

Graphene-based flexible Hall sensors

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Since the seminal work of Novoselov et al., there has been a great effort to make use of the superior electronic properties of graphene [1]. Graphene-based applications in large-area electronics require reliable and scalable production of uniform films of graphene. Among many methods hitherto developed, chemical vapor deposition (CVD) has emerged as the most feasible strategy for the synthesis of large sheets of uniform graphene films [2]. Having low density of charge carriers with high mobility, graphene is a favorable material for the manufacture of Hall devices [3, 4]. Moreover, it is suitable for flexible electronic applications, thanks to its flexibility and tensile strength [5]. For such applications, transfer-printing of graphene via lamination onto polymeric substrates was successfully performed [6,7,8]. Laminating graphene-on-copper obtained via atmospheric-pressure CVD with 75μm PVC film, we developed a simple and low-cost scheme for the fabrication of graphene-based flexible Hall generators, without resorting to metallization techniques such as evaporation or sputtering. Instead of these techniques, electrical contacts are provided by the pieces of copper foils preserved during the chemical etching with an aqueous solution of ferric chloride. By using this scheme, we fabricated cross-shaped Hall generators having active areas of 1x1, 2x2, 3x3, 4x4, 5x5, and 10x10 mm^2. The resistances and Hall coefficients of the devices are ~1 kΩ and ~-100 V/(A·T). The thickness of the copper foil used in the fabrication is 15 μm and thus the thickness of the devices is 90 μm. It is evident that the thickness of the device is mainly determined by the thickness of the flexible substrate. Therefore, thinner devices could be fabricated by utilizing thinner flexible substrates.

[1] K. S. Novoselov et al., *Science Vol. 306, Issue 5696, pp. 666-669* (2004).

[2] X. Chen et al., Synthetic Metals 210 (2015) 95–108

[3] Chiu-Chun Tang et al., Appl. Phys. Lett. 99, 112107 (2011).

[4] S. Sonusen et al., Applied Surface Science 308 (2014) 414–418.

[5] Changgu Lee et al., *Science* Vol. 321, Issue 5887, pp. 385-388 (2008).

[6] Sukang Bae et al., Nature Nanotechnology 5, 574–578 (2010).

[7] Luiz G. P. Martins et al., Proceedings of the National Academy of Sciences of the United States of America, 17762–17767 (2013).

[8] E. O. Polat et al., *Scientific Reports* **4**, Article number: 6484 (2014).

Please indicate your preference:

Oral Presentation: [X]

Multilayer Graphene Based Passive Matrix OLED Displays

Süleyman Çelik[1], Hasan Özkaya[1], Sibel Kasap[1], Taylan Erol[1] and Ismet I. Kaya[1,2]

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[2]Sabancı University, Faculty of Engineering and Natural Sciences, Istanbul/Turkey

Graphene is one of the most promising candidate materials for display technology due to its conductivity, optical transparency and unmatched flexibility. However, in spite of its theoretical potential, practically graphene still falls short of ITO to be implemented in the industry. Some of the technical handicaps are lower conductivity/transparency, non-uniformity, and controlling of the surface contamination and roughness. In this presentation we will report demonstration of passive matrix monochrome OLED displays with 1” size and up to 200 dpi resolution in which multilayer graphene films were utilized as the anode electrodes. Graphene films were synthesized by CVD on nickel and then transferred onto glass as well as flexible substrates by PMMA supported wet transfer method. We will demonstrate the results and discuss the yield and efficiency issues with the graphene based displays and compare their performance to ITO based displays.

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Epitaxial Graphene Contact Electrode for Optoelectronics Device Applications

Erdi Kuşdemir, Dilce Özkendir, Damla Yeşilpınar, Batuhan Kalkan, Cem Çelebi

Izmir Institute of Technology, Department of Physics, Quantum Device Laboratory

*Presenter: cemcelebi@iyte.edu.tr

Graphene is considered to be used as transparent conductive electrode for next generation optoelectronics devices such as photodetectors and photovoltaic solar cells, due to its superior electrical conductivity and mechanical flexibility. Unlike other optically transparent conductors including ITO, Ni/Au, Ti and Ti/W, graphene has excellent optical transparency with a 90% transmittance level for the 200 - 400 nm wavelength spectral region.

Because of its high UV transmission level and zero band gap, graphene has become a promising candidate to be used as conductive and transparent electrode especially for UV sensitive photodetectors. It is known that one atom thick graphene layer can be grown readily on a UV sensitive SiC semiconductor crystal by epitaxial growth techniques without using any deposition and/or transfer process.

In our study, single layer epitaxial graphene template with great thickness uniformity was grown on a SiC semiconducting substrate by using high temperature ultra-high vacuum annealing process. We fabricated and characterized a novel graphene-semiconductor-graphene (GSG) type UV sensitive device based on the rectifying character of the Schottky junction formed at the epitaxial graphene/SiC interface. The fabricated GSG device (shown in the figure) consists of 20 optically transparent graphene finger electrodes. The performance of our GSG sample was characterized both in the absence and in the presence of 254 nm wavelength UV light. The samples with graphene finger electrodes revealed the typical I-V characteristics of a conventional metal-semiconductor-metal (MSM) type photodetector with low leakage current, excellent photocurrent reversibility and high response speed. The experimentally obtained results imply that epitaxial graphene can be used readily as transparent conductor especially for SiC based optoelectronic device applications.

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Poster Presentation: [ ]

2016 Graphene & Related Materials Conference (GRM-2016)

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2016 Graphene & Related Materials Conference (GRM-2016), Ankara, Turkey
July 13-15, 2016

Atomic collapse in graphene

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The chiral nature of charge carriers in graphene prohibits backscattering and prevents confinement by electrostatic potentials, resulting in high electronic mobility and unusual phenomena such as Klein tunneling [1]. This picture breaks down in the presence of charge impurities exceeding a critical value Z_c, where a qualitative change in behavior leads to the capture of electrons akin to atomic collapse in 3D atoms. Although in graphene Z_c is substantially lower than in 3D atoms, attaining the supercritical regime is difficult because screening can significantly reduce the effective charge of the impurity.

The transition from sub-critical to the supercritical regime is accompanied by trapping of electrons in quasi-bound states which are the condensed matter analogue of the long sought after phenomenon of atomic collapse in super-heavy nuclei. The quasi-bound electron-states show up as a strong enhancement of the density of states within a disc centered on the vacancy site. We find that these states are surrounded by a circular halo of hole states which are interpreted as the analogue of positron production in atomic collapse [2]. We further show that the quasi-bound states at the vacancy site are gate tunable and that the trapping mechanism can be turned on and off, providing a new paradigm to confine, control and guide electrons in graphene.

We found that a sharp STM tip is able to induce similar atomic collapse states. For large tip potentials a sub-micrometer scale p-n junction is induced that exhibits whisper gallery modes. When the tip is positioned close to an edge we observe Fabry-Perot resonances of the electronic waves.

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A Mechanical Chain Reaction on Graphene at a Substrate Edge

G. Özbal[1], J. T. Rasmussen[2], M. Brandbyge[2] , R. T. Senger[1] , H. Sevinçli[3]

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Thanks to its exotic and rich features, research on graphene-related materials systems still continues. In recent years, detailed analyses have been performed on the stability of hydrogen clusters on flat graphene [1–3]. In this study we reconsider the energetically most preferable configurations of hydrogen atoms on graphene from dimers to hexamers. All calculations are performed by means of density functional theory (DFT) and density functional based tight binding (DFTB) methods. Unlike previous studies, in this study we have come across a general trend towards forming a linear chain and armchair pattern which we attribute to sp^2 hybridization in graphene turning into a pseudo-sp^3 hybridization with the adsorbed hydrogens. The main purpose of this study is investigating the curvature effect on hydrogen configurations formed on graphene by examining the relative total energies of hydrogen families. This goal is achieved by bending the graphene with natural angle 52-degree at substrate edge which arises from the pseudo-sp^3 hybridization. It is well-known that curvature alters the reactivity of graphene markedly and it is shown that when the hydrogen atoms are ordered as linear chains the reaction barrier is reduced approximately 15% for realistic cases [4]. In our study several configurations are well-tested in the form of families and generations. Our findings point out that binding energies of hydrogens on flat graphene are lower than those of curved graphene. Furthermore linear chain reaction occurs from pseudo-sp^3 and curvature effect spontaneously. It should be noted that, armchair pattern becomes dominant as the number of additional hydrogen atoms increases.

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Oral Presentation: [X]

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Adsorption and diffusion on new two dimensional carbon allotropes (graphyne)

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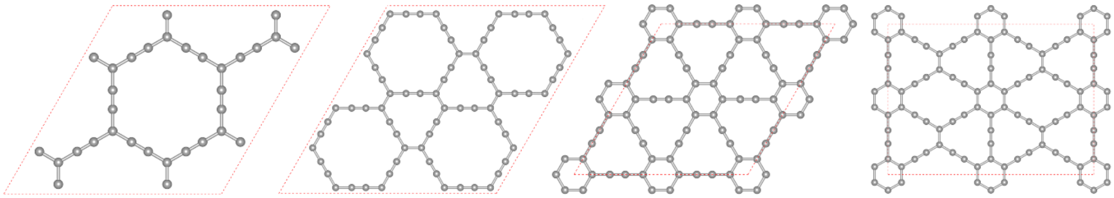
Carbon exhibits various forms of hybridization (sp, sp2, sp3) and has many allotropes including graphite, fullerene, nanotube and graphene. Among them, two dimensional (2D) graphene attracted much interest from experimental and theoretical side because of its remarkable mechanical (hardness, the strongest material) and electronic properties (Dirac cone, high electron mobility). These remarkable properties made graphene a novel material for future carbon-based electronics. This also motivates the research on other 2D carbon based materials. Beyond graphene (pure sp2), the new 2D carbon allotropes the so-called graphyne, containing sp and sp2 hybridization on carbon atom, have been envisioned [1-7].



In this study, we systematically the studied single atom adsorption (H, O, N, and S) on four graphyne polymorphs (α-, β-, γ- and 6612) by using first principles techniques. Firstly, we have tested possible binding sites such as bridge, top and hollow sites for each polymorph. While oxygen, nitrogen and sulfur atoms prefer in-plane sites, H binds on top of carbon atoms. Next, we have studied the resulting electronic structure for ground state configurations. The adsorption generally transfroms α-, β- and 6612 graphyne from semi-metal to semiconductor. And finally, we have analyzed the lateral diffusion of adsorbed atoms on α- and γ-graphyne polymorphs. The calculated energy barriers are very high indicating that atoms cannot move on the surface.

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Please indicate your preference:

Oral Presentation: [x]

Tunable Optoelectronic Properties of Graphene by Charge Doping

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The unique electronic and optical properties of graphene due to the linear dispersion of Dirac electrons provide basis for a wide range of applications; such as optical detectors, modulators and displays with tunable broadband optoelectronic properties. We have investigated the electronic and optical properties of single layer graphene from first principles, by doping electrons or holes as homogeneous background charge. The electronic bandstructure, i.e. the energy range of permitted interband electronic transitions as well as the onsets of optical absorption were observed to be modified by differing carrier concentrations. Modifying incrementally the electron or hole concentration led to a regular blue or redshift of the optical conductivity onsets. These shifts can be directly related with the altered Fermi energy levels relying on the allowed band-to-band electronic transitions within the doped systems. Therefore, it is possible to control the interband transitions within the visible and ultraviolet wavelength regime, by increasing or decreasing the carrier concentrations in graphene. This research was supported by TUBITAK (project no. 113T050).

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A Facile Method for Clean Graphene Transfer Based on Sacrificial Photoresist Layers

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Chemical vapor deposition of graphene on copper or other metal foils such as nickel has attracted great interest in recent years. However, transfer of graphene from such substrates is still a challenge, due to problems with tears, wrinkles and cleanliness. The most common method for such transfers is the wet transfer method based on poly(methyl methacrylate)-PMMA sacrificial layers, which displays problems because of PMMA's fragility and difficult removal from above graphene. Here we demonstrate a method based on a common photoresist, replacing PMMA. By simple drop casting without spinning, the photoresist forms a thick layer above graphene, preventing fragility and enabling easy fish-out process from the metal-etch solvent. The resist layer can also can be removed easily by acetone, not requiring extensive high temperature annealing under hydrogen.

This work has been supported by the Scientific and Technological Research Council of Turkey (TUBITAK) (Project # 115F014).

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Poster Presentation: [ ]

The Influence of Interface Size and Topography on the Nanotribology of Graphene: A Combined Experimental and Numerical Study

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Two-dimensional (2D) materials have been the focus of intense research in recent years thanks to their outstanding electronic and mechanical attributes. In particular, graphene exhibits exceptional potential as a solid lubricant appropriate for use in nano-/micro-scale mechanical systems. As such, a comprehensive evaluation of its frictional properties on such small length scales is of crucial concern. While pioneering studies toward this purpose have revealed strongly layer-dependent frictional behavior [1], the precise roles that interface size and topography (important design parameters for mobile components in nano-/micro-scale devices) play in the lubricative nature of graphene have not been explored yet in detail.

In this contribution, we present a combined experimental and numerical study aimed at evaluating the influence of interface size and topography on the nanotribological characteristics of graphene. In particular, atomic force microscopy (AFM) is employed under ambient conditions to measure friction forces on mechanically-exfoliated graphene as a function of applied load, number of graphene layers, and interface size. To study the influence of interface size on measured frictional properties, AFM probes with different tip apex sizes are obtained by thermal evaporation of gold and platinum onto the probes. In conjunction with the experiments, molecular dynamics (MD) simulations are performed that involve the calculation of friction forces experienced by model tip apexes of varying size on single- and few-layer graphene. Moreover, substrates with various RMS roughness and correlation length values are employed in the MD simulations to investigate the effect of substrate topography on frictional behavior. Results reveal that a subtle interplay between probe size and substrate topography determines the layer-dependent frictional behavior of graphene, providing a new perspective to the nanotribology of this remarkable material.

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Please indicate your preference:

Oral Presentation: [X]

Friction of Graphene over 4H-SiC{0001} Surfaces

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Nanotribological properties of graphene has been subject to numerous studies in recent years due to its potential in providing exceptional friction control in various applications and a deeper understanding of the nature of friction. The exact origins of various observed phenomena related to the friction of graphene at the nanoscale such as ultralow friction (superlubricity) [1] , the dependence of the friction coefficient on the number of layers [2-3] or the effect of substrate morphology [4] are yet to be fully understood. We investigated the frictional properties of graphene on a silicon carbide substrate from first principles by conducting a density functional theory based study of sliding graphene layers on 4H-SiC{0001} surfaces. Sliding of single and multiple graphene layers over the 4H-SiC{0001} surfaces along different directions and under various computational constraints is examined. It is observed that upon sliding the interaction between the surface and graphene layers alternates between van-der Waals and covalent interactions which dramatically affects friction. We determine the friction coefficients under low loads and analyze the variations in the electronic structure during sliding. Single or multiple graphene layers were displaced along armchair (x) and zig-zag (y) directions under various normal loads. The sliding profiles were extracted through optimization of the systems at each step over a dense mesh along the sliding paths. We present a force-based model to determine friction coefficients and compare our results with experimental data. Upon further inspecting the electronic structure, we provide insight into the underlying mechanisms of friction.

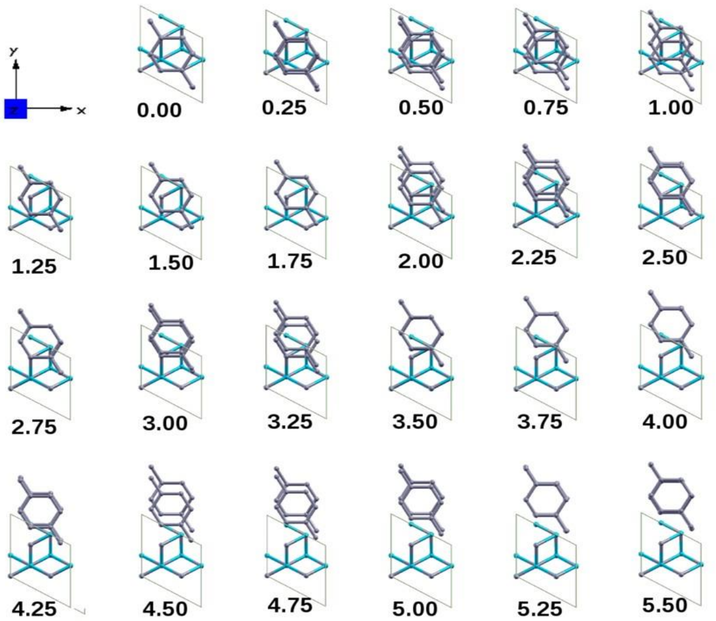

Figure: Optimized geometries at each step in sliding bi-layer graphene along zig-zag direction on the 4H-SiC(000-1) surface.

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Oral Presentation: [X]

Graphene Quantum Devices

P. Simonet, H. Overweg, M. Eich, D. Bischoff, A. Varlet, T. Ihn and K. Ensslin

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Graphene quantum devices are potential candidates for spin qubits because of predicted long spin coherence times. Graphene quantum dots show Coulomb blockade, excited states and their orbital and spin properties have been investigated in high magnetic fields. Most quantum dots fabricated to date are fabricated with electron beam lithography and dry etching which generally leads to uncontrolled and probably rough edges. We demonstrate that devices with reduced bulk disorder fabricated on BN substrates display similar localized states as those fabricated on the more standard SiO2 substrates. A way to overcome edge roughness and the localized states related to this are bilayer devices where a band gap can be induced by suitable top and back gate voltages. By placing bilayer graphene between two BN layers high electronic quality can be achieved as documented by the observation of broken symmetry states in the quantum Hall regime. In addition a Lifshitz transition can occur indicating a tunable topology of the Fermi circle. This can be exploited to achieve smoother and better tunable graphene quantum devices.

Electronic transport experiment in graphene allow for experiments where both classical and quantum mechanical charge detector back-action on a quantum dot are investigated. Two stacked graphene quantum dots separated by a thin layer of boron nitride lead to quantum systems closer to each other than it is possible for conventional 2D systems. By applying a finite bias to one quantum dot, a current is induced in the other unbiased dot. The observed measurement-induced current is based on strong capacitive coupling and energy dependent tunneling barriers, breaking the spatial symmetry in the unbiased system. This is a special feature of graphene-based quantum devices. The experimental observation of transport in classically forbidden regimes is understood by considering higher-order quantum mechanical back-action mechanisms.

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Atomic and Island Scale Diffusion Events on Bi_2Te_3 (0001) Surface

Mert Taşkın[1], Dilek Yıldız[1,2], Carl Willem Rischau[3], Cornelis J. Van der Beek[3], Alberto Ubaldini[4] and Oğuzhan Gürlü[1*]

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[2] Department of Physics, University of Basel, Basel, Switzerland
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[4]Département de Physique de la Matiére Condensée, Université de Genéve, Geneva, Switzerland

Bi_2Te_3 consists of quintuples, which contain five atomic planes (Te1-Bi-Te2-Bi-Te1), and the interfaces of quintuples have weak van der Waals bonds between them [1]. Cleaving a Bi_2Te_3 crystal at the (0001) plane results in a Te1 terminated surface. In this work morphology of this surface was investigated by Scanning Tunneling Microscopy (STM) under ambient conditions. We observed mainly two defect types, which appeared as vacancy defects (Figure-a) and clover shaped charge localizations (Figure-b). We investigated the diffusion of vacancy defects on these surfaces by time-lapse STM imaging. Diffusion of vacancy defects occur on Te1 terminated (0001) surface laterally or along c-axis. We calculated jump rate of vacant sites for lateral diffusion. Vacant sites were observed to coalesce to form vacancy islands. At larger scale vacancy islands coarsen via Ostwald Ripening. Relation between mean radius of a vacancy island (R) and observation time (t) is exponential, $R \sim t^n$, where exponent n characterize the diffusion mechanism [2]. Our data revealed that vacancy islands coarsen by $n \sim 1/3$, which in turn indicated that they grow mainly by evaporation of vacancies at their edges [2]. Further measurements show that other diffusion mechanisms may have a role in coarsening of the vacancy islands.

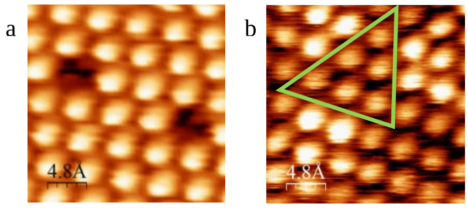

Figure: STM Topography Images of Te1 surface of Bi_2Te_3. a) Bright spots correspond to Te atoms while dark sites are assumed to be due to vacancies (V_{tip}=550 mV, I_t=250 pA). b) Charge localization on topmost layer marked by a green triangle (V_{tip}=500 mV, I_t=250 pA).

This work was supported by a TUBITAK-CNRS bilateral project with grant number 113F005 and a TUBITAK 1003 project with grant number 114F036.

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Please indicate your preference:

Oral Presentation: [X]

Poster Presentation: [ ]

Photon Emission from Graphene/Copper Interface in a Tunnel Junction

H. Tunç Çiftçi [1], Berk Zengin[1], Umut Kamber[1], Cem Kıncal[1], Dilek Yıldız[1,2], M. Selman Tamer[1] and Oğuzhan Gürlü [1*]

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Developments in scanning probe microscopy techniques paved the way to study photon emission (PE) phenomena with lateral resolution on surfaces [1]. Tunneling electrons, which are injected from the tip of a scanning tunneling microscope (STM) to a surface may result in the emission of photons from the tunnel junction. Such photon emission can be due to the optical-radiative decay of the localized surface plasmons (LSP), which can be excited by the tunneling injected electrons to the surface. In this work, PE properties of graphene/copper system due to tunneling injected electrons have been investigated using a home-built, ambient photon-STM (Figure-1.a). Detailed analysis of pSTM measurements showed that photons are emanating from Cu(111) facets beneath graphene layer, which indicated the existence of a free electron like surface at the graphene/copper interface.

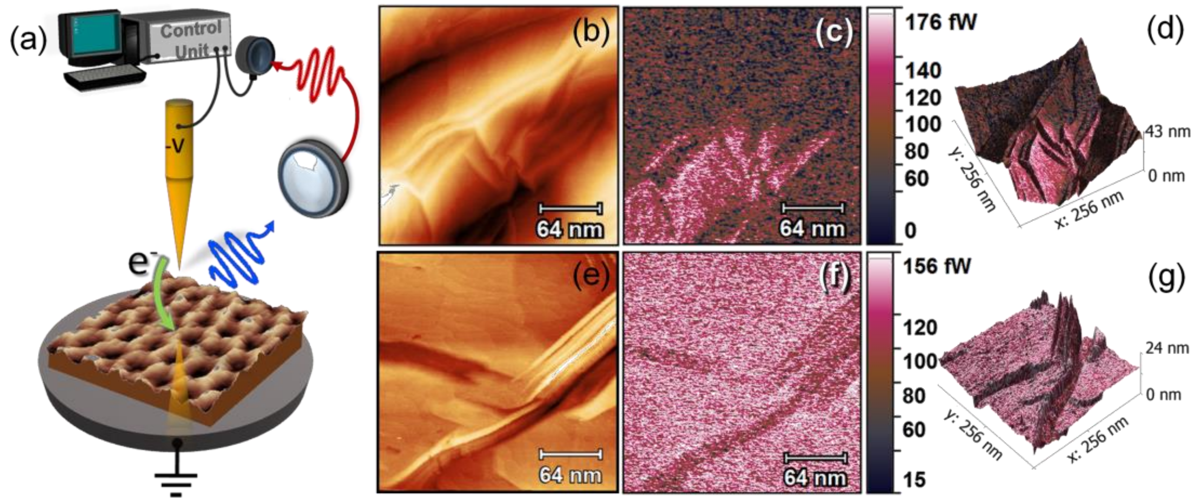

Figure-1 (a) Home-built, ambient pSTM. (b,e) Simultaneously taken topography and (c,f) photon maps. (d,g) Facet dependency of PE is illustrated by overlapping photon maps on topography.

This work was supported by TUBİTAK 1003 project with grant number 114F036.

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Please indicate your preference:

Oral Presentation: [x]

Poster Presentation: [ ]

Swift Heavy Ion Irradiation of Graphene Layers on HOPG

Cem Kıncal[1], Dilek Yıldız[1,2], Mert Taşkın[1], Clara Grygiel[3], Cornelis J. van der Beek[4] and Oğuzhan Gürlü[1]

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Unzipping and folding of graphene layers on dielectric substrates were shown to be possible by swift heavy ion (SHI) irradiation under grazing incidence [1]. However, origin of the unzipping behavior of graphene on dielectric substrates was not understood. In such experiments, possible effect of the dielectric substrate cannot be neglected. To understand substrate effect we proposed SHI irradiation of moiré zones on HOPG due to the fact that moiré zones may partially behave like dislocated graphene films on its native substrate [2].

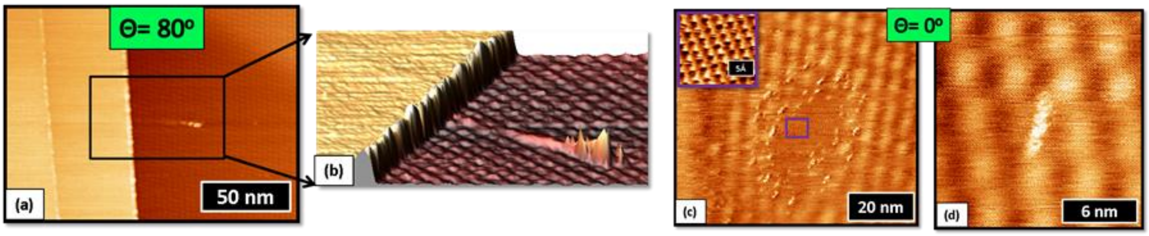

Figure: (a) Large-area and (b) zoom-in STM images of SHI induced comet-like structures on a moiré zone on HOPG surface. (c) Locally removed moiré zone on upon SHI irradiation and (d) SHI induced defect on another moiré zone on the same sample. (Tunneling Parameters: (a,b) V= 300mV, I= 0.4nA, (c) V= 50mV, I= 0.5nA and (d) V= 50mV, I= 0.4nA)

Our results showed that SHI irradiation of moiré zones on HOPG surfaces under grazing incidence did not show any unzipping of the graphene generating the moiré patterns. The defects forming as a result of grazing incidence irradiation of moiré zones were comet-like similar to SHI induced defects on pristine HOPG surfaces. On the other hand, we observed that perpendicularly irradiated moiré zones can either be locally defected as the HOPG terrace or they can be removed locally at a larger scale. In this presentation behavior of varying moiré zones upon SHI irradiation will be discussed. This work was supported by a TÜBİTAK-CNRS-2505 bilateral project with grant number 113F005.

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Please indicate your preference:

Oral Presentation: [x]

Poster Presentation: [ ]

Comparative Scanning Tunneling Microscopy Study of Self-Assembled Alkanethiol Monolayers on Highly Oriented Pyrolytic Graphite and Single-Layer Graphene

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The recently discovered *wonder material* graphene has attracted considerable attention from the scientific community due to its outstanding physical properties [1]. Among a large variety of proposed applications, graphene-based chemical sensors are especially promising due to the fact that graphene's electronic properties readily change upon adsorption of particular atomic/molecular species on its surface [2]. On the other hand, the fact that graphene consists of carbon atoms held together by strong covalent bonds leads to the outcome that it exhibits weak chemical interactions with other atoms and molecules in its vicinity, severely hampering its applicability in chemical sensors.

Motivated by the issue outlined above, it has recently been proposed that the graphene surface can be *functionalized* with self-assembled monolayers (SAMs) of a specific alkanethiol (1-octadecanethiol) that displays particular affinity toward heavy metal ions for chemical sensing applications [3]. On the other hand, the effect of (i) using different alkanethiol molecules and (ii) the number of graphene layers on the molecular structure and electronic properties of the SAMs –and therefore their effectiveness in chemical sensing– has not been studied in detail.

In this contribution, to investigate the molecular structure associated with SAMs formed by alkanethiol molecules as a function of molecular size and number of graphene layers, we designed a comparative scanning tunneling microscopy (STM) study. In particular, we image SAMs formed by 1-octadecanethiol (ODT, $C_{18}H_{38}S$) and 1-dodecanethiol (DDT, $C_{12}H_{26}S$) on highly oriented pyrolytic graphite (HOPG) and single-layer graphene grown by chemical vapor deposition (CVD) using a *Nanosurf EasyScan 2* instrument with high resolution under ambient conditions. Results of STM imaging experiments reveal the different self-assembly patterns associated with alkanethiol structures formed on HOPG and graphene. The different molecular arrangements observed for SAMs formed on HOPG and single-layer graphene by the same organic molecule (DDT) point toward the influence of number of graphene layers, and therefore, varying degrees of adsorbate-substrate interactions on molecular self-assembly.

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Oral Presentation: [X]

2016 Graphene & Related Materials Conference (GRM-2016)

Bilkent University, Ankara, Turkey

July 13-15, 2016

Oral Presentations

July 15, Friday

Graphene Based Tunable Photonic Metamaterials

Ekmel Özbay

Nanotechnology Research Center, Bilkent University, Bilkent, 06800 Ankara, Turkey

In this talk, we will present how we can integrate metamaterials and graphene to obtain tunable nanophotonic structures. We obtained resonance broadening and tuning of split ring resonators by utilizing an epitaxial graphene transistor with transparent top-gate. Metallic split ring resonator (SRR) structures are used in nanophotonics applications in order to localize and enhance incident electromagnetic field. Electrically controllable sheet carrier concentration of graphene provides a platform where the resonance of the SRRs fabricated on graphene can be tuned. The reflectivity spectra of SRR arrays shift by applying gate voltage, which modulates the sheet carrier concentration, and thereby the optical conductivity of monolayer graphene. We experimentally and numerically demonstrated that the tuning range can be increased by tailoring the effective mode area of the SRR and enhancing the interaction with graphene. We also demonstrated a graphene-based device with ionic liquid gating and V-shaped plasmonic antennas to both enhance and more effectively tune the total optical response.

Large conductance fluctuation and localization in suspended monolayer graphene

Vahid Sazgari[1,2], Cenk Yanik[1,2], Abdulkadir Canatar[1,2], Yaser Vaheb[2], Ismet I. Kaya[1,2]

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Conductance fluctuations (CF) has been widely studied in electron systems. They originate from the interference between phase-coherent electrons propagating in all possible paths through a mesoscopic system. In conventional semiconductors and metals, the average amplitude of these fluctuations is a universal number of the order of e^2/h giving rise to UCF. In graphene, however, due to its unique band structure, the fluctuations of the conductance is highly dependent on the geometry of the device [1], and the spatial distribution [2] as well as the strength of the scattering potentials in a disordered system [3]. Therefore, unlike the conventional 2D electron systems, CF in graphene can cross over between non-universal and universal regimes depending on the system size and the disorder strength. It has been shown that in the limit of very large size and disorder strength, the CF becomes universal whereas for more realistic sample parameters it is in a non-universal crossover regime [3].

Here, we have investigated the large conductance fluctuations of a thermally cycled highly cleaned suspended monolayer graphene. As the temperature is lowered, the quantum transport of electrons becomes coherent leading to quantum interference corrections to the conductance. We observed that by lowering the temperature the fluctuations of conductance is strongly pronounced reaching the average amplitude of $\sim e^2/h$ at lowest temperatures. As shown in Fig. 1, the fluctuations are also reproducible at different temperatures and becomes so strong at lower temperatures that they can even suppress the conductance occasionally around the Dirac point leading to an insulating behavior when the carriers are totally localized in the bulk.

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Oral Presentation: [x]

Theoretical Investigation of Conductance and Quantum Capacitance of Quantum Hall Effect Edge states

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In this work we investigate edge states of two dimensional electron system (2DES) in quantum Hall (QH) regime[1]. We consider scattering and temperature effects on density of states of 2DES. Under magnetic field Landau Levels (LL) are broadened due to these temperature and scattering. Density of states of 2DES defined as two different model, first one is Gaussian model[2], second one is self consistent Born approximation (SCBA), which has semi eliptic form for describe extended and localized states[3]. Also quantum capacitance concept, which is equal to density of states of 2DES, investigated for QH regime. Edge states of QH regime divided by two region under magnetic field, which are called compressible and incompressible strips. Compressible strips act as metallic and screens confinemet potential and incompressible strips acts as insulator has poor screening properties[4]. Recent experiment about edges of QH regime shows conductance values depend on total capacitance of system and resistance of 2DES[5]. We calculated numerically this conductance and quantum capacitance expressions for exact experiment conditions with respect to Thomas Fermi Poisson approximation and our result shows similar result with experiment.

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<u>Please indicate your preference:</u>

Oral Presentation: [X]

Electronic and Spintronic Properties of Disordered Zigzag Graphene Nanoribbons

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Properties of graphene nanostructures deviate from bulk graphene due to quantum confinement and edge effects. Graphene nanoribbons, confined in one direction has been under strict investigation mainly because energy gap opening and theoretically proposed induced magnetism along the zigzag edges in agreement with Lieb's theorem [1]. This property makes ZGNRs a perfect candidate for microelectronic and spintronic devices [2,3]. In this study, we have theoretically compared the effect of long and short range impurity potentials on the electronic, magnetic properties of ZGNRs. For long range fluctuations, we observed that electron interaction effects make edge states robust against disorders and if the disorder is strong enough a magnetic phase transition from antiferromagnetic to ferromagnetic coupled edges occur [4]. However, these kind of impurities protect the sublattice symmetry and leads to phenomena known as "absence of backscattering" which give rise to minimum conductivity on graphene. On the other hand, in order to model hydrogenation effects, we used short range impurity potential which breaks the sublattice symmetry. Using a time dependent tight binding model, we observed Anderson localization induced metal to insulator transition with a nanometer scale localization length for 2% hydrogen coverage. We found that, Anderson localization is stronger at high energy valence states since those states are more vulnerable to hydrogenation [5].

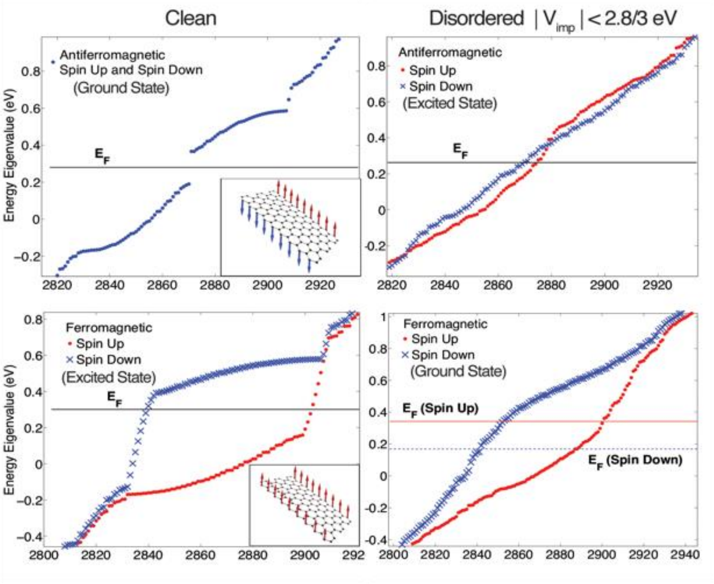

Fig. 1. Mean-field Hubbard spectra for antiferromagnetic (top panels) and ferromagnetic (bottom panels) phases, E_F spin up and spin down show the spin-dependent Fermi levels.

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Oral Presentation: [X]

Controlled Perforation of Freestanding Graphene by Focused Ion and Electron Beams

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Due to its extraordinary mechanical properties, microscale free-standing graphene can withstand several bars of pressure differences, making it a promising new material for water purification and gas separation applications. Scientifically, graphene pores also provide a novel platform to study mass permeation through nanopores with sub-nm thickness. However, it is not easy to control the perforation of graphene in order to obtain narrow pore diameter distribution. Using focused ion and electron beams, and optimizing particularly the ionic current and the electron exposure times, we have demonstrated effective pore diameter control down to sub-5-nm. Transport characterization of these pores display ballistic gas transport, which is also important for the fundamental studies of nanoscale mass transport.

This work has been supported by the Scientific and Technological Research Council of Turkey (TUBITAK) (Project # 115Y302).

<u>Please indicate your preference:</u>

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Poster Presentation: [ ]

2016 Graphene & Related Materials Conference (GRM-2016), Ankara, Turkey
July 13-15, 2016

Large Area Monolayer Graphene Oxide Synthesis by Controlled Oxidation

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Chemical exfoliation of graphene or graphene oxide (GO) from graphite has become the method of choice for mass-scale production purposes. However, it is not easy to control the thickness and lateral size of the final flakes due to irregular oxidation and exfoliation of graphite. Hence, the probability of obtaining few-layer or thicker flakes is higher compared to other non-chemical methods to obtain graphene. Here, we demonstrate a simple method to control the oxidation reactions and enhance interlayer intercalation of graphite during the early stages of graphite oxidation. The produced flakes display monolayer thickness and lateral dimensions reaching up to tens of microns.

This work has been supported by the Scientific and Technological Research Council of Turkey (TUBITAK) (Project # 115Y302).

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Structural and Optical Properties of Hexagonal Boron Nitride Thin Films Deposited by Sequential Exposures of Triethylboron and N_2/H_2 Plasma

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Hexagonal boron nitride (hBN) growth is a matter of technological and scientific interest due to its useful properties such as large band gap, high thermal conductivity, high oxidation resistance, and low surface energy. Previously halide precursors such as BF_3, BCl_3 and BBr_3 have been utilized for atomic layer deposition of hBN. However, a key limitation associated with these halide precursors is their by-products which are corrosive and hazardous.[1] Alternatively, borazine has been employed as a CVD precursor for the growth of hBN, but surface-inhibited growth has been reported owing to the inertness and low surface energy of hBN surface.[2][3]

In this work, we demonstrate the low-temperature CVD growth of BN using triethylboron and N_2/H_2 plasma as boron and nitrogen precursors, respectively. The sequential injection of these precursors potentially offers highly-predictable synthesis of BN with accurate sub-nm level thickness control defined by growth parameters. Effect of growth parameters such as substrate temperature, precursor pulse and purge times, and number of cycles on deposition rate and resulting film composition and structure are presented. The resulting films deposited at 350 and 450 °C were found to have nano-crystalline wurtzite crystal structure and the high-resolution XPS scans confirmed the BN formation. Optical characterization showed a refractive index value of ~1.65 along with an optical band-edge around 5.3 eV.

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<u>Please indicate your preference:</u>

Oral Presentation: [X]

2016 Graphene & Related Materials Conference (GRM-2016)

Bilkent University, Ankara, Turkey

July 13-15, 2016

Poster Presentations

Electron-Zone Boundary Phonon Interactions in Graphene: Effect of Haldane-like Mass

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Haldane [1], in 1988, introduced a model exhibiting important properties on a graphene lattice. Its significance of Haldane mass comes from the the fact that it generates the quantum Hall effect in graphene without magnetic fields, that breaks parity as well as time-reversal symmetry. Haldane mass term is different from the gaps generated by the Kane-Mele type topological mass term, intrinsic mass term, and conventional mass term. It is simply a staggered on-site energy, which is taken to have different signs on each sites. The interaction is represented by a mass term and it is related to the realization of the parity anomaly in (2+1) dimensional relativistic field theory. It is also well know that effects of electron-phonon interaction on graphene in the presence of spin-orbit interaction is a crucial issue since it enables the manipulation of the spin of charge carriers that leads to a new generation of spin-based nano devices [2]. The effects of both intrinsic and Rashba spin orbit couplings in graphene were examined in [3,4]. In this study, we examine the interaction of graphene charge carriers with optical A_{1g}-phonons in the presence of Rashba spin-orbit interaction together with a Haldane mass term. A Fröhlich type Hamiltonian is considered to describe the electron-phonon system within the continuum limit. It is shown that electron-A_{1g} phonon interactions strongly affects the gapped graphene electronic structure in the presence of Rashba-type spin-orbit interaction.

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Please indicate your preference:

Poster Presentation: [X]

Optical Properties of Graphene Quantum Dots

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We investigate theoretically the optical conductance of clean and disordered graphene quantum dots (GQD) consisting of up to 10806 atoms [1]. The calculations are performed within tight binding and mean field Hubbard approximations where the imperfections in the GQD are modeled using a random potential landscape. The optical conductance of GQD is found to be very close to the universal optical conductance of isolated monolayer of graphene sheet given by $(\pi/2)*e^2/h$ [2,3]. We find that the disorder induced electron and hole localizations near Fermi level is reduced due to electron-electron interactions making the observation of universal optical conductance robust against imperfections.

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Please indicate your preference:

Poster Presentation: [X]

The magnetic anisotropy in single-layer crystal structures

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The effect of an applied electric field and the effect of charging are investigated on the magnetic anisotropy (MA) of various stable two-dimensional (2D) crystals such as graphene, $FeCl_2$, graphone, fluorographene, and $MoTe_2$ using first-principles calculations. We found[1] that the magnetocrystalline anisotropy energy of Co-on-graphene and Os-doped-$MoTe_2$ systems change linearly with electric field, opening the possibility of electric field tuning MA of these compounds. In addition, charging can rotate the easy-axis direction of Co-on-graphene and Os-doped-$MoTe_2$ systems from the out-of-plane (in-plane) to in-plane (out-of-plane) direction. The tunable MA of the studied materials is crucial for nanoscale electronic technologies such as data storage and spintronics devices. Our results show that controlling the MA of the mentioned 2D crystal structures can be realized in various ways, and this can lead to the emergence of a wide range of potential applications where the tuning and switching of magnetic functionalities are important.

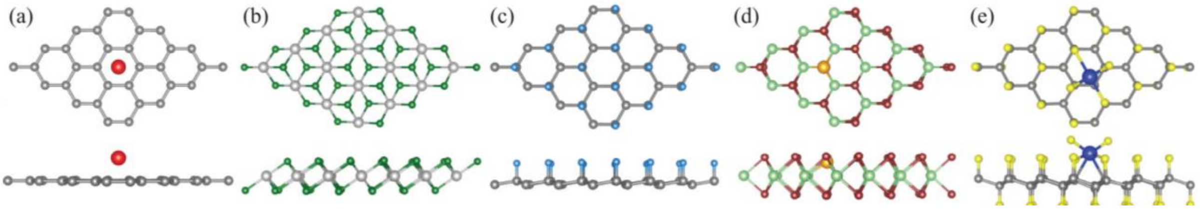

Fig. 1 *(a) Co on graphene. Co and C atoms are shown in red and dark gray, respectively. (b)* $FeCl_2$ *in a 1T structure. Fe and Cl atoms are shown in light gray and green, respectively. (c) Graphone. C and H atoms are shown in dark gray and blue, respectively. (d) Os-doped* $MoTe_2$ *. Mo, Te, and Os atoms are shown in light green, red, and orange, ctively. (e) V on fluorographene. F, C, and V atoms are shown in yellow, dark gray, and blue, respectively.*

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<u>Please indicate your preference:</u>

Poster Presentation: [X]

Hexagonal AlN: Indirect-to-direct Band GapTransition

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Motivated by a recent experiment that reported the successful synthesis of hexagonal (*h*) AlN [Tsipas et al., Appl. Phys. Lett. 103, 251605 (2013)], we investigate[1] structural, electronic, and vibrational properties of bulk, bilayer, and monolayer structures of h-AlN by using first-principles calculations. We show that the hexagonal phase of the bulk *h*-AlN is a stable direct-band-gap semiconductor. The calculated phonon spectrum displays a rigid-layer shear mode at 274 cm^{-1} and an E$_g$ mode at 703 cm^{-1}, which are observable by Raman measurements. In addition, single-layer *h*-AlN is an indirect-band-gap semiconductor with a nonmagnetic ground state. For the bilayer structure, *AA*-type stacking is found to be the most favorable one, and interlayer interaction is strong. While N-layered h-AlN is an indirect-band-gap semiconductor for N = 1−9, we predict that thicker structures (N≥10) have a direct band gap at the *Γ* point. The number-of-layer-dependent band-gap transitions in *h*-AlN is interesting in that it is significantly different from the indirect-to-direct crossover obtained in the transition-metal dichalcogenides.

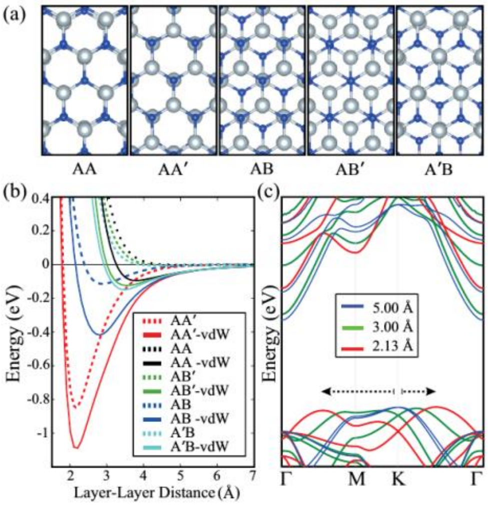

Fig 1. *(a) Possible stackings between two layers of h-AlN. (b) Layer-layer interaction energy for different stackings. (c) Interlayer-spacing-dependent band dispersion of AA stacked two layers of h-AlN.*

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Please indicate your preference:

Poster Presentation: [X]

Bilayer SnS_2: Tuning the stacking order

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Employing density functional theory–based methods, we investigate[1] monolayer and bilayer structures of hexagonal SnS_2, which is a recently synthesized monolayer metal dichalcogenide. In its bilayer structure we examine different stacking configurations of the two layers. It is found that the interlayer coupling in bilayer SnS_2 is weaker than that of typical transition-metal dichalcogenides so that alternative stacking orders have similar structural parameters and they are separated with low energy barriers. A possible signature of the stacking order in the SnS_2 bilayer has been sought in the calculated absorbance and reflectivity spectra. We also study the effects of the external electric field, charging, and loading pressure on the characteristic properties of bilayer SnS_2. It is found that (i) the electric field increases the coupling between the layers at its preferred stacking order, so the barrier height increases, (ii) the bang gap value can be tuned by the external E-field and under sufficient E-field, the bilayer SnS_2 can become a semimetal, (iii) the most favorable stacking order can be switched by charging, and (iv) a loading pressure exceeding 3 GPa changes the stacking order. The E-field tunable band gap and easily tunable stacking sequence of SnS_2 layers make this 2D crystal structure a good candidate for field effect transistor and nanoscale lubricant applications.

[1] C. Bacaksiz, S. Cahangirov, A. Rubio, R. T. Senger, F. M. Peeters, and H. Sahin. Phys. Rev. B **93**, 125403 (2016).

Please indicate your preference:

Poster Presentation: [X]

Piezoelectric Performance of BN Dopped Graphene Ribbons

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After the invention of the extraordinary properties of the graphene, such as high electrical conductivity and mechanical strength, a way opened to use it as a stretchable transparent electrode [4], ballistic transistor, etc. Besides these attractive properties, graphene has a limitation in application of electronic devices because of forbidden energy range lack. Hexagonal boron nitride (h-BN) layers are isostructural with graphene and also have nearly the same lattice parameters. Unlike graphene, h-BN structures have quite high forbidden energy gap. So, doping graphene layer with h-BN will break centrosymmetry and allows the formation of energy gap. Piezoelectricity is another notable property of 2D materials, which is an unique property of non-centrosymmetric structures with sufficiently high energy gap, with wide variety of applications, pressure sensors, transducers, high voltage generators, nonlinear energy harvesters and piezotronics . Last years, researchers interest focused on to give piezoelectric property to graphene.

In this study, systematic investigation of the electronic and piezoelectric properties of BN doped six different graphene ribbons investigated theoretically via first principles calculations. Besides electronic properties, elastic stiffness constants (C_{11} and C_{12}), Young modulus (Y), Poisson's ratios(v), piezoelectric stress (e_{11}) and piezoelectric strain (d_{11}) coefficients are calculated. Our results reveal that the width of the BN changes the piezoelectric performance of graphene ribbons which can be comparable with conventional piezoelectrics.

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Please indicate your preference:

Poster Presentation: [X]

Development of Graphene/Carbon Fiber Hybrids Electrocatalyst for PEM Fuel Cells

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Consideration of being taken into account for the design of a fuel cell catalyst is the high surface area. This target has to be realized by dispersing catalyst phase in a conductive support which usually being used carbon [1]. For this purpose, the utilization of nano-structured carbonaceous materials as support present as promising solution for fuel cells. However, for enhancing the catalytic activity and stability is to increase the interaction between Pt and its supports, in order to inhibit the tendency of Pt nanoparticle coalescence [2].

In this study, for providing the aforementioned carbon support system, a hybrid carbon fiber and graphene oxide was prepared by hydrothermal treatment and microwave method. As seen on Fig. 1 before the experiment GaquA [3] and graphene oxide were dispersed in water (a) but after treatment all materials precipitated (b). Also, Raman spectrum (c) shows us that D band (ID) and G band (IG) peaks were decreased. This proves us that the functional groups on graphene oxide and carbon fiber reduced both under high temperature and high pressure conditions.

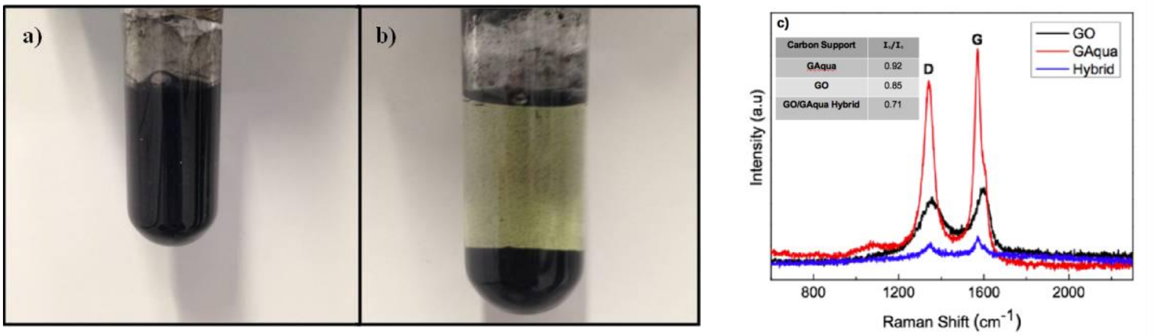

Fig.1. GAquA and GO hybrid carbon materials (a) before and (b) after treatment in microwave oven (c) Raman spectrum of the hybrid catalyst support

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Please indicate your preference:

Poster Presentation: [X]

Fabrication of Ultra-Clean Suspended Graphene Devices

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Graphene, a single layer of carbon atoms, has attracted enormous attention due to its relativistic nature and interesting physical properties. Although theoretical studies on graphene are quite successful and revealing many interesting results about Dirac-like condensed matter systems, experimental realizations of these predictions are very challenging. Due to the naturally occurring electron-hole puddles and impurities acquired during the fabrication, graphene devices merely show their true potential, i.e. physics at the Dirac point [1]. In order to achieve an ultra-high quality graphene device with less impurity concentration and higher carrier mobility, graphene sheets are whether suspended [2] or placed on an atomically flat hBN layer [3], both of which reduce electron-hole puddles and lead ultra-high carrier mobility graphene samples. While putting graphene sheet on hBN breaks inversion symmetry due to its periodic potential [4], suspended graphene shows the full graphene properties without any modification in its physics.

Here, we introduce our techniques for fabricating ultra-clean, high mobility suspended monolayer graphene devices in order to make Dirac point more accessible and reach the best graphene samples. We will present our fabrication and cleaning techniques (i.e. current annealing), which lead us to produce devices with charge mobility values in excess of 10^6 cm^2/V-s. We will show some of our data revealing the improvement in graphene quality after current annealing and its implications.

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Please indicate your preference:

Poster Presentation: [x]

Effect of disorder on transport through graphene antidot lattice

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Abstract We study the effect of disorder on the electronic transport in graphene antidot lattices (GAL). It was shown that introducing a periodic array of antidots, graphene can have a finite band gap [1]. Recently, electronic transport in GAL with disorder is investigated by using Kubo-Greenwood formalism and it was found that while disorder removes the band gap, it opens a transport gap caused by Anderson localization [2]. In our calculations, Non-Equilibrium Green's Function (NEGF) method is used. We define the Hamiltonian of the system composed of two semi-infinite electrodes and one central (scattering) region in block-tridiagonal form using the tight-binding model with nearest neighbour interactions. We consider no interaction between layers and neglect electron-electron interactions. The decimation method [3] is utilized in the calculation of Green's function of the central part. Sancho-Rubio recursive scheme [4] is used in the calculation of self energies of the electrodes, which in turn allows us to calculate the Green's Function of the whole system and the desired quantities such as density of states, electrical conductance and mean free paths. Further, we focus on the relation between disorder and dimensionality in asymmetric lattices.

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Please indicate your preference:

Poster Presentation: [X]

STABILITY OF TWO DIMENSIONAL (2D) STRUCTURES BASED ON GaAs

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Graphene is a two dimensional material isolated for the first time in 2004 by mechanical exfoliation from graphite. After this, two dimensional materials attract a lot of attention, and become one of the most studied and explored material system because of their various exotic properties. In this study, we searched for new stable 2D structures formed by Ga and As atoms based on GaAs structure or its functionalized form with O atoms. In search for such a system, we performed density functional theory based calculations by using a plane-wave pseudopotential method. First, we performed geometrical optimization calculations in order to identify possible stable structures. Then, we calculated the phonon dispersions in order to check the mechanical stability of these structures. Eventually, we obtained electron band diagrams and investigate their electronic properties.

<u>Please indicate your preference:</u>

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Effects and Effectiveness of Various Organic Solvents on PMMA-Based Transferred Graphene Films

Taylan Erol[1], Sibel Kasap[1], Suleyman Celik[1], Abdulkadir Canatar[2], Ismet I. Kaya[1,2]

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The most common and well established method of graphene transfer is done by supporting the graphene film by poly(methyl methacrylate) PMMA and it is well known that removal of PMMA layer from graphene film is a challenging task due to strong interactions between PMMA and graphene that stems from local rehybridization of carbon atoms from sp^2 to sp^3 [1]. Here we present the results of an experimental study to determine the effects and effectiveness of four different solvents that are commonly used to remove PMMA from the surface of CVD grown graphene. The effectiveness of the solvents was determined by measuring the residual coverage using atomic force microscopy. The results demonstrate that removal of PMMA from the graphene surface is in good correlation with its Hansen solubility in the respective solvent. N-methyl-2- pyrrolidone is found to be the most effective in removal of poly(methyl methacrylate) PMMA layer from graphene film than other chosen organics solvents, which are acetone, acetic acid and chloroform. Raman mapping analysis revealed that partial removal of PMMA from graphene surface induced local strain that is correlated with the amount of residue.

[1] Y. Han, *et al*., J. Mater. Chem. C. 2 (2014) 201–207. doi:10.1039/C3TC31722F.

<u>Please indicate your preference:</u>

Poster Presentation: [x]

Large Area Graphene Synthesis via Hydrothermal Method

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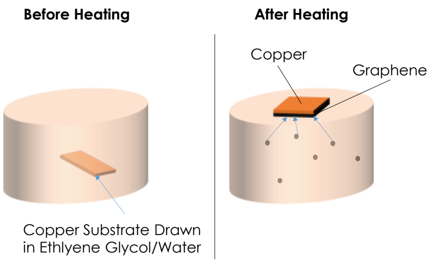
Graphene, unlike to conventional Chemical Vapor Deposition (CVD), is synthesized via hydrothermal method on large area uniformly on copper substrate. Produced structure has very good uniformity by means of layer thickness and good continuity on plane.

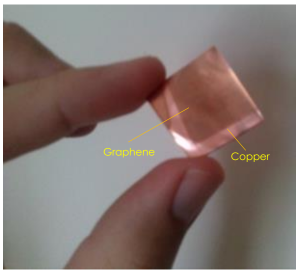
Between 190-250°C, hydrothermal synthesis in autoclave was pursued with Ethylene Glycol in water with 1M, which act as Carbon source. No inert gas or constant pressure is required in the process. Since Hydrogen to Carbon ratio is 3 for Ethylene Glycol ($C_2H_6O_2$), according to reference [1], it is suitable to use it for hydrothermal synthesis of Graphene. Also Copper substrate acts as a catalyst to speed up Graphene formation. Chrome oxide autoclave walls also covered with copper foil to increase the growth yield.

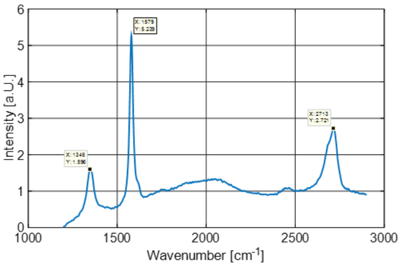
Since Graphene is hydrophobic, Copper/water interface is highly beneficial to collect Graphene, which sticks very tightly on Copper foil.

Synthesized Graphene

Defects, that are visible under Raman spectroscopy, would be possibly arisen because of impurities inside liquid source. Peak around 1350 cm^{-1} at Raman spectrum shows that synthesized structure has relatively low defects [2]. Growing mechanism and Raman spectrum (right) could be seen in following Figure.







[1]. L. Tang, et al., J. Mater. Chem.,22, 5676-5683 (2012).

[2]. A. Ferrari et al., Physical Review Letters 97, p. 187401 (2006).

Please indicate your preference:

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Poster Presentation: [X]

Single Layer TiS$_3$: Vacancy Formation and Oxidation

F. Iyikanat[1], R. T. Senger[1], F. M. Peeters[3], H. Sahin[2]

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In this study, the structural, electronic, and magnetic properties of pristine, defective, and oxidized monolayer TiS$_3$ are investigated using first-principles calculations in the framework of density functional theory.[1] We found that a single layer of TiS$_3$ is a direct band gap semiconductor, and the bonding nature of the crystal is fundamentally different from other transition metal chalcogenides. The negatively charged surfaces of single layer TiS$_3$ makes this crystal a promising material for lubrication applications. The formation energies of possible vacancies, i.e. S, Ti, TiS, and double S, are investigated via total energy optimization calculations. We found that the formation of a single S vacancy was the most likely one among the considered vacancy types. While a single S vacancy results in a nonmagnetic, semiconducting character with an enhanced band gap, other vacancy types induce metallic behavior with spin polarization of 0.3−0.8 μ_B . The reactivity of pristine and defective TiS$_3$ crystals against oxidation was investigated using conjugate gradient calculations where we considered the interaction with atomic O, O 2 , and O 3 . While O 2 has the lowest binding energy with 0.05−0.07 eV, O 3 forms strong bonds stable even at moderate temperatures. The strong interaction (3.9−4.0 eV) between atomic O and TiS 3 results in dissociative adsorption of some O-containing molecules. In addition, the presence of S-vacancies enhances the reactivity of the surface with atomic O, whereas it had a negative effect on the reactivity with O2 and O3 molecules.

[1] F. Iyikanat, H. Sahin, R. T. Senger, and F. M. Peeters, J. Phys. Chem. C **119**, 10709 (2015).

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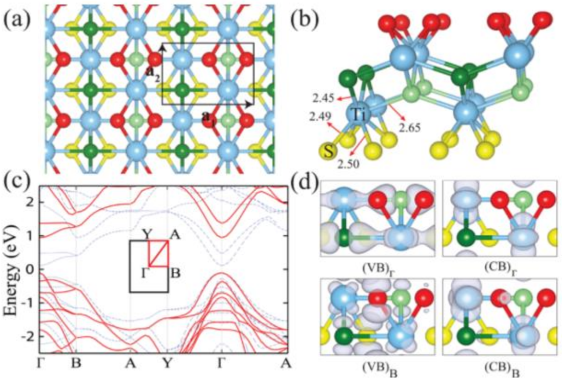

Figure 1. (a) Top view of monolayer TiS$_3$ and its unit cell shown by a rectangle. For a better top view, S atoms in different layers are presented by different colors. (b) Tilted side view of 2 × 2 × 1 supercell of monolayer TiS$_3$. (c) Blue dashed lines and red lines illustrate PBE and HSE06 results for the electronic band diagram of monolayer TiS$_3$, respectively. (d) Band decomposed charge densities of valence band (VB) and conductance band (CB) at Γ and B.

Diffusion Characteristics of Ag and Au Atoms Intercalated in Bilayer Heterostructures

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In this study, we investigated the diffusive motion of metal nanoparticles Au and Ag on monolayer and between bilayer heterostructures of transition metal dichalcogenides and graphene in the framework of density functional theory.[1] We found that the minimum energy barriers for diffusion and the possibility of cluster formation depend strongly on both the type on nanoparticle and the type of monolayers and bilayers. Moreover, the tendency to form clusters of Ag and Au can be tuned by creating various bilayers. Tunability of the diffusion characteristics of adatoms in van der Waals heterostructures holds promise for controllable growth of nanostructures.

[1] F. Iyikanat, H. Sahin, R. T. Senger, F. M. Peeters, APL Mater. **2**, 092801 (2014)

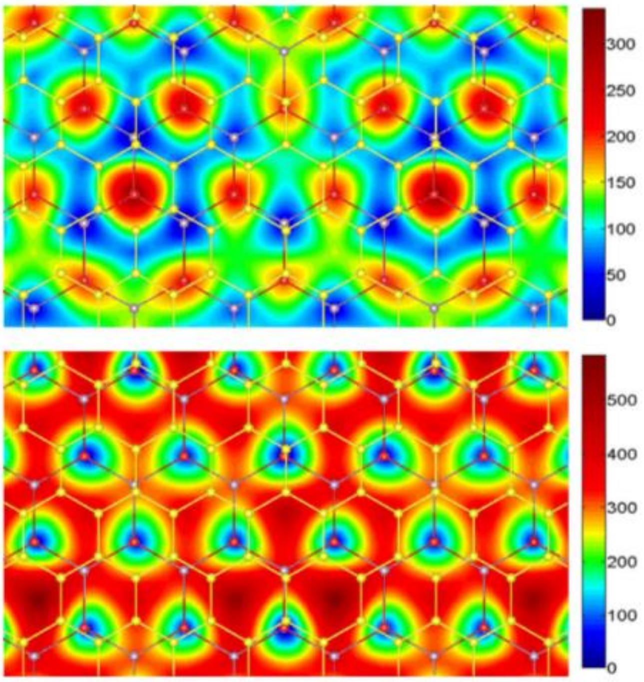

FIG. 4. Contour plots of the energy barriers (in meV units) seen by Ag (upper panel) and Au (lower panel) atoms intercalated in MoS_2/Graphene heterostructure.

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Bulk, Bilayer, and Monolayer Structures of Portlandite Crystal

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[1]Department of Physics, Izmir Institute of Technology, 35430, Izmir, Turkey
[2]Department of Photonics, Izmir Institute of Technology, 35430, Izmir, Turkey
[3]Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium
[4]School for Engineering of Matter, Transport and Energy Arizona State University, Tempe Arizona, 85287, USA

$Ca(OH)_2$ crystals, well known as portlandite, are grown in layered form, and in the recent study we found that they can be exfoliated on different substrates.[1] We performed first principles calculations to investigate the structural, electronic, vibrational, and mechanical properties of bulk, bilayer, and monolayer structures of this material. Different from other lamellar structures such as graphite and transition-metal dichalcogenides, intralayer bonding in $Ca(OH)_2$ is mainly ionic, while the interlayer interaction remains a weak dispersion-type force. Unlike well-known transition-metal dichalcogenides that exhibit an indirect-to-direct band gap crossover when going from bulk to a single layer, $Ca(OH)_2$ is a direct band gap semiconductor independent of the number layers. The in-plane Young's modulus and the in-plane shear modulus of monolayer $Ca(OH)_2$ are predicted to be quite low while the in-plane Poisson ratio is larger in comparison to those in the monolayer of ionic crystal BN. We measured the Raman spectrum of bulk $Ca(OH)_2$ and identified the high-frequency OH stretching mode A_{1g} at 3620 cm^{-1} . In this study, bilayer and monolayer portlandite [$Ca(OH)_2$] are predicted to be stable and their characteristics are analyzed in detail. Our results can guide further research on ultrathin hydroxites.

[1] Y. Aierken, H. Sahin, F. Iyikanat, S. Horzum, A. Suslu, B. Chen, R. T. Senger, S. Tongay, and F. M. Peeters, Phys. Rev. B **91**, 245413, (2015).

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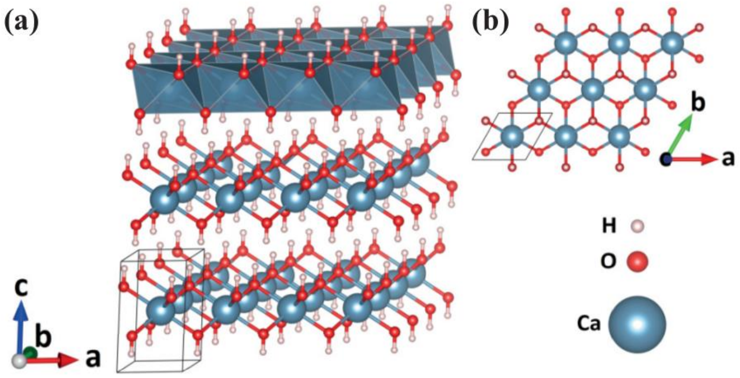

FIG. 1. (Color online) Atomic structure of bulk $Ca(OH)_2$: (a) tilted view, (b) top view of one layer.

2016 Graphene & Related Materials Conference (GRM-2016), Ankara, Turkey
July 13-15, 2016

Electronic, Magnetic, and Transport Properties of Monolayer MoS_2 with Grain Boundaries

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In this study, the structural, electronic, magnetic and transport properties of monolayer MoS_2 are investigated with a focus of various type of grain boundaries using the first principle calculations. Considered grain boundaries consist of different misorientation angles and diverse defect types. The geometric stabilities of grain boundaries are calculated and compared with the pristine MoS_2. The electronic properties of monolayer MoS_2 show diversity in the presence of grain boundaries. Considerable amount of magnetic moment observed on the Mo atoms in the vicinity of grain boundaries. Moreover, the electronic transport through these grain boundaries is investigated and our results show that the conductance properties of MoS_2 near to the band gap edges are quite sensitive to the misorientation angle and the defect type of grain boundary. The impact of the magnetic moment of grain boundary dominates the conduction properties of MoS_2. These results could be useful for designing future applications in nanoelectronics and spintronics.

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Investigation of Graphene using Simultaneous Scanning Tunneling/Atomic Force Microscopy

Majid Fazeli Jadidi, Umut Kamber, Oğuzhan Gürlü, Hakan Özgür Özer
Istanbul Technical University, Department of Physics Engineering, Istanbul, 06469, Turkey

We investigated graphene layers grown on Cu foils using simultaneous Scanning Tunneling Microscopy/Atomic Force Microscopy (STM/AFM). Atomic resolution images of the surface were obtained in many channels such as STM topography, oscillation amplitude, force, tunnel barrier height and phase shift. The simultaneous acquisition of multiple channels allows us to compare images at every pixel, which in turn sheds light on the contrast mechanisms in probe microscopy. Force-distance spectroscopy is also carried out with acquisition of such channels. The results suggest a very strong repulsive interaction between the tip and sample atoms during ordinary STM operating conditions on graphene.

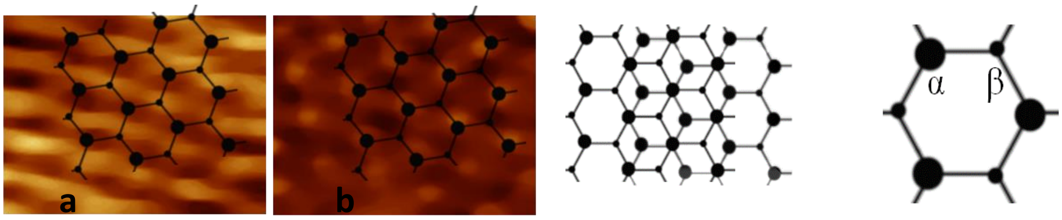

Figure-1: Simultaneous STM/AFM images of graphene surface: (a) STM topograph (b) Oscialltion amplitude Si cantilever. $k \cong 50$ N/m. f= 47 kHz. 15 x 15 $Å^2$, $V_{sample} = 0.2$ V, $I_t = 0.17$ nA, $A_0 = 0.56$ $Å_{rms}$. Hexagonal lattice model is overlaid on the images.

Figure 1. shows simultaneously acquired STM topography and oscillation images of the surface using a Si cantilever. The three atoms of the hexagonal cell appear higher than the other three. In HOPG or multilayer graphene, due to the shift between two successive layers, 3 atoms of the hexagon have an atom underneath (alpha (A) site) whereas the other 3 don't have (beta (B) site). Hence three main atomic structures at the surface are A and B atoms and hollow sites. In STM images B atoms appear higher due to the dominance of their electronic structure over A site atoms. The model of the hexagonal lattice is overlaid on the images for clarity. In the oscillation amplitude images which is a measure of the interaction stiffness [1], the brighter spots match with the A sites. The oscillation amplitude throughout the entire image is well below the free amplitude which suggests a very high positive interaction stiffness. This observation is supported also by the F-d and I-d curves which are simultaneously acquired.

The support by TÜBİTAK through grants 114F036 and 109T679 is gratefully acknowledged.

Corresponding author: oozer@itu.edu.tr

[1] A. Oral, R. A. Grimble, H. Ö. Özer, P. M. Hoffmann, and J. B. Pethica, Appl. Phys. Lett. 79, 1915 (2001).

<u>Please indicate your preference:</u>

Poster Presentation: [x]

Friction Force Microscopy Study on Fractal Structures at the Graphene-Copper Interface

Umut Kamber, Cem Kıncal and Oğuzhan Gürlü

Istanbul Technical University, Faculty of Sciences and Letters, Department of Physics,
34469, Maslak, Sarıyer, İstanbul, Turkey

Chemical Vapor Deposition (CVD) became a widely employed method to produce graphene on metal foils, since produced graphene can easily be transferred onto another substrates [1]. By changing the conditions of CVD process, we discovered controlled ways to produce dendritic and point-like silicon-oxide structures on our samples. Such structures were observed both on graphene/Cu-foil system and also on pure Cu-foils after CVD processes. We investigated whether these interesting particles formed at the graphene/Cu interface or on the graphene layer using Friction Force Microscopy (FFM). We studied friction properties of CVD-grown graphene near and on silicon-oxide fractals. We also performed FFM measurements on silicon-oxide structures forming on pure Cu-foils [2]. Results of FFM measurements on our samples gave us valuable information to understand the formation mechanism of dendritic structures as well as their whereabouts on the graphene/Cu system.

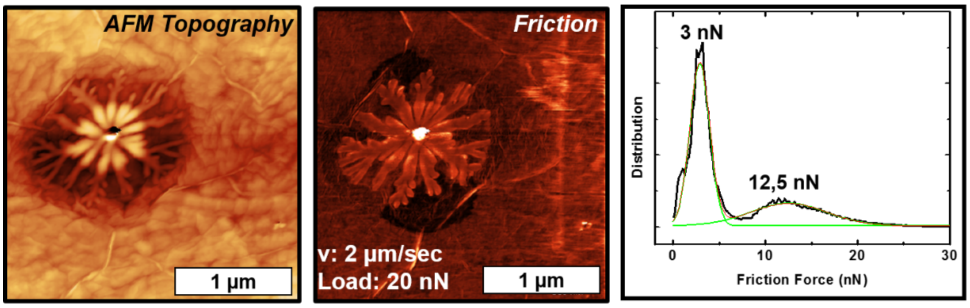

Figure: AFM topography of silicon-oxide fractal on graphene/Cu-foil and corresponding friction force map. Histogram shows friction force distribution of the scanning area.

This work was supported by TÜBİTAK-1003 project with grant number 114F036.

[1] Li, X., et al., Science, 324 (5932), 1312-1314 (2009)

[2] U. Kamber et al., *Lateral Force Microscopy study on silicon-oxide fractals at Graphene-Copper Interface.* (submitted) (2016).

Please indicate your preference:

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Poster Presentation: [x]

Density Functional Tight Binding Parametrization for Single Layer MoS_2

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[*]Department of Materials Science and Engineering, Izmir Institute of Technology,
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Two-dimensional form of graphite, graphene has paved a novel way in nano-science and nano-technology to reveal the potential of the other two-dimensional (2D) form of materials. Transition metal dichalgonides (TMDs), a family of novel 2D materials, have been attracting a lot of interest due to their variety of novel properties and device functionalities. As the first discovered member of the family, a monolayer of molybdenum disulfide (MoS_2) has remarkable optical and electronic properties[1]. Density functional theory (DFT) is the most powerful and widely used method in computational materials science. Its power is mainly due to its predictive power and its ability to compute large systems, which would not be possible otherwise. Density functional tight binding (DFTB) method, on the other hand, enhances the computational limits by combining the speed of tight binding methodology with the accuracy of DFT[2]. We developed a self consistent charge (SCC) DFTB parameter set for Mo and S which yields electronic band structure of single layer MoS_2 successfully. With this new parameter set, it is possible to model realistic defect and grain boundary structures. Here, we present our results on complex unit cells of defective MoS_2.

[1] Wang Q.H., Kalantar-Zadeh K., Kis A., Coleman J.N., Strano M.S., *Nature Nanotechnology*, **7**, 699-712, 2012.

[2] Koskinen P., Makinen V., *Computational Materials Science*, **47**, 237-253, 2009.

Please indicate your preference:

Poster Presentation: [X]

Solvent Effect on the Quantum Capacitance of Graphene-Based New Generation Supercapacitors

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The properties of graphene-based supercapacitors are investigated from first principles calculations based on density functional theory (DFT). In order to improve their energy storage capacity, combination of both electrode and electrolyte are examined. Bilayer graphene is used as electrode materials and ammonium as electrolyte in our supercapacitor models. In our calculations, plane wave pseudo-potential method and both the local density approximation (LDA) and van der Waals functional for exchange-correlation potential are used. We started with the adsorption of ammonia on monolayer graphene. The different configurations (hollow (H), top (T) and bridge (B)) and orientations (up and down) of NH_3 on monolayer graphene are scrutinized. Bridge case is found to be the most energetically favorable. Supercapacitors are created from bilayer systems. The quantum capacitances of the models are calculated based on density of states (DOS) (Figure 1). The density effect of ammonium in graphene bilayer is studied to investigate the concentration effect on the final capacitance calculation in solvent medium. The effect of the solvent environment on the electronic structure and the quantum capacitance of the graphene based supercapacitor systems have been studied using the nonlinear polarizable continuum model. Solution results are compared with the vacuum results. In addition, doping effect and vacancy defect on the capacitance of supercapacitors are examined.

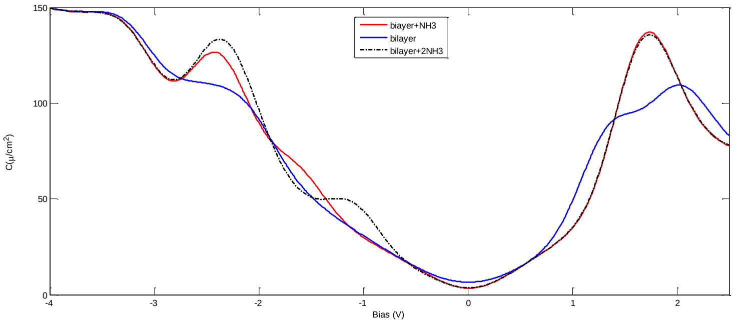

Figure 1. The quantum capacitances of the graphene based supercapacitor systems

This work is supported by TÜBİTAK Project No: 114F118

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Synthesis of Three-Dimensional Graphene Foam for Nuclear Waste Management Applications

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Disposal of ^{90}Sr and ^{137}Cs from aqueous solutions, the main fission by-products of spent fuels, is one of the most important issues to protect environmental safety in nuclear waste management since they have relatively long half-life which is about 30 years. Adsorption is a highly selective and efficient process frequently used to filter these materials in nuclear waste management. However, existing adsorbents such as resins, clays, polymers, micro- and nano-metal oxides and carbon based materials suffer from lower capacity and operational problems. Therefore, there is a growing need for new and better performing adsorbent systems.

Three-dimensional (3D) graphene-based frameworks in the form of aerogels, hydrogels, sponges and foams are new-generation carbon materials. Among them, graphene foam has appeared to be a promising and important prospect owing to its micro- and macro-porous structure, low density and large surface area. The aim of this study is to investigate the capability of 3D graphene foam to remove strontium and cesium ions from aqueous solutions by adsorption process. Graphene foams were grown on metal foam by chemical vapor deposition process. The performance assessment will be done by sorption experiments under batch and continuous flow conditions in a fixed bed mode.

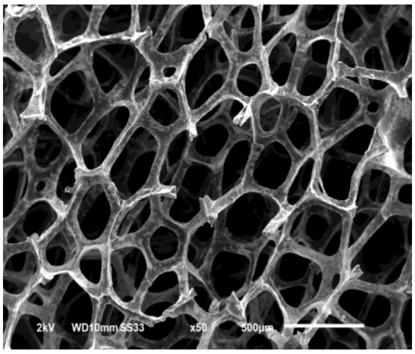

Figure. SEM image of a graphene foam grown by CVD.

[1] Chen,Z., Ren, W., Gao, L., Liu, B., Pei, S., Cheng, HM., 2011, “ Three dimensional flexible and conductive interconnected graphene networks grown by chemical-vapor deposition”, Nature materials.

[2] Cao, X., Shi, Y., Shi, W., Lu, G., Huang, X., Yan, Q., Zhang, Q., 2011, “Preparation of novel 3D graphene networks for supercapacitor application”, Small.

Poster Presentation: [x]

Electronic and Optical Properties of New Emerging Two-dimensional Group-VA Arsenene from Many-body Calculations

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[1]UNAM-National Nanotechnology Research Center, Bilkent University, Ankara, Turkey
[2]Institute of Materials Science and Nanotechnology, Bilkent University, Ankara, Turkey
[3]Department of Physics, Bilkent University, Ankara, Turkey

Lately, due to the growing demand on new classes of two-dimensional materials in broadband optoelectronic device applications, LEDs and photovoltaics, accurate calculation of their electronic and optical properties has gained great importance. Starting from layered 3D crystalline phase of arsenic, we performed an extensive analysis on the structural, mechanical, electronic and optical properties of single-layer buckled and washboard arsenene and their bilayers using density functional and many-body perturbation theories. While 3D layered gray arsenic crystal is a semimetal, single-layer (SL) and bilayer (BL) arsenene phases are semiconductors, where fundamental band gaps decrease with increasing layer number. We have also investigated the influence of the thickness of 2D systems and biaxial tensile strain, which were observed to tune the spectral (optical) properties of Arsenene; hence could be noteworthy parameters for their solar cell applications. The light absorption of SL and BL As structures in general falls within the visible-ultraviolet spectral regime. Directional anisotropy, adding extra layers and applying homogeneous or uniaxial in-plane tensile strain can alter the optical properties aimed for diverse photovoltaic and optoelectronic applications. Beyond the random-phase approximation, the excitonic effects were also accounted for by undertaking the Bethe-Salpeter formalism, where evidence of a strongly bound exciton was not traced. We belive that this study highlights the significance of the prospective realization of layered (2D) forms of Group VA Arsenene aimed for optoelectronic applications, especially within the solar energy regime. This research was supported by TUBITAK (project no. 115F088).

<u>Please indicate your preference:</u>

Poster Presentation: [x]

2016 Graphene & Related Materials Conference (GRM-2016), Ankara, Turkey
July 13-15, 2016

Effect of methane pressure on average size of graphene crystals in chemical vapour deposition (CVD) on copper

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[2]Nanotechnology Research and Application Center, Sabanci University, Istanbul, Turkey

In recent years CVD growth of graphene on copper revealed great prospective for large area production and high crystalline quality. However despite of various progresses, this method is still suffer from different challenges such as production costs and inadequate sheet conductance for some applications. In this regard, the average crystalline size plays critical role on characteristics of graphene film produced by CVD. As it known, presence of impurities and surface defects on the copper increases nucleation centers and consequently decreases graphene crystals sizes and sheet conductance as well. Therefore usage of highly purified copper foil is a common approach to achieve best possible quality for graphene film, though it dramatically raises production cost. In such a condition, optimizing growth parameters to restrict nucleation rate can provides desired graphene quality on commercially available copper foils, which is more favorable.

In this work to study average size of graphene crystals we terminate the CVD growth before full coverage of graphene on copper surface, accordingly there will be a clear color contrast in low energy electron microscopy images between bare copper surface and those parts which covered by graphene. In this way we can monitor size and shape of crystal patches as well as their nucleation density. Using this method we are tracing the effect of methane flow rate and its partial pressure. So far we managed to enhance more than one order of magnitude average size of graphene crystals by decreasing nucleation density as a result of decreasing methane partial pressure.

<u>Please indicate your preference:</u>

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Friction Force Microscopy studies on swift heavy ion irradiated graphitic surfaces

Cem Kıncal[1], Dilek Yıldız[1,2], Umut Kamber[1], Mert Taşkın[1], Clara Grygiel[3], Cornelis J. van der Beek[4] and Oğuzhan Gürlü[1]

[1] Department of Physics, Istanbul Technical University, Istanbul, Turkey
[2] Department of Physics, University of Basel, Basel, Switzerland
[3] Centre Interdisciplinaire Ions Matériaux et Photonique, Caen, France
[4]Laboratoire des Solides Irradiés, Ecole Polytechnique, Palaiseau, France

Scanning probe microscopy has been useful in investigating track formations on surfaces due to swift heavy ion (SHI) irradiation under grazing incidence. Comet-like structures on SHI irradiated HOPG surfaces under grazing incidence were previously reported in STM studies [1]. Our results confirm the comet-like track formations on HOPG surfaces due to SHI irradiation. We have shown that it was possible to obtain atomic resolution on the tail section of the comet-like structures. Such STM data proved that the interaction of SHI with the bulk does not damage surface layers.

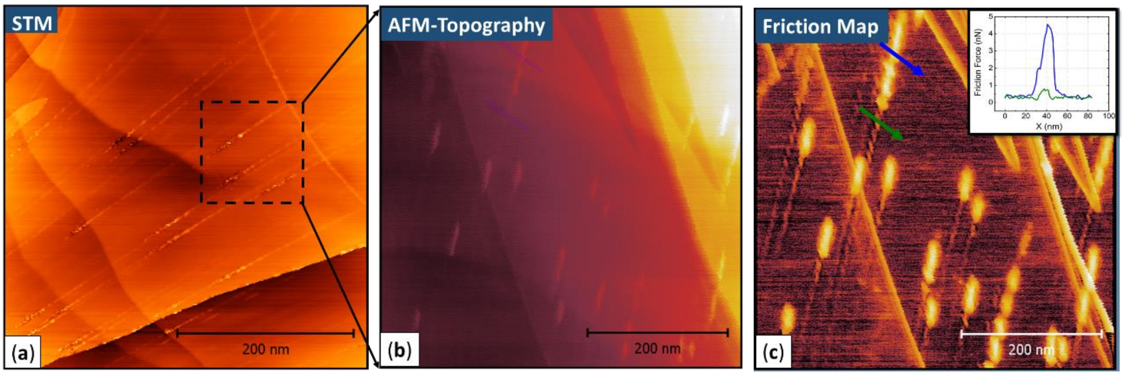

Figure: (a) Large-area STM image of SHI induced comet-like structures on HOPG, (b) Contact mode AFM topography image of same sample, (c) simultaneously measured friction force map. (Tunneling Parameters: V= 300mV, I= 0.4nA, Load force: 20nN for (b,c))

Our friction force microscopy measurements showed complementary results to our STM measurements. Intriguingly we observed that the tail-sections of the comet-like structures appeared in friction force maps (Figure-c), although they could not be seen in the simultaneously taken topography maps (Figure-b). This work was supported by a TÜBİTAK-CNRS-2505 bilateral project with grant number 113F005.

[1] J. Liu et al., Nucl. Instr. and Meth. in Phys. Res. B **193**, 259 (2002).

Please indicate your preference:

Oral Presentation: [ ]

Poster Presentation: [x]

Reversible Thermal Switch Based on Photoisomerism

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The form of energy, carried by lattice vibrations(phonons), named as heat, has been considered as waste energy. However, controlling and understanding heat flow in crystals would provide opportunities to build nano thermal devices. The aim of this work is to design a thermal switch, which is based on photoisomerism. Reversible photoisomerism is a key ingredient in molecular junctions, where a single molecule is placed between two electrodes. In this work, we use azobenzene, one of photoisomeric molecules that changes its three-dimensional structure when exposed to UV radiation, which could form a basis for light-driven molecular thermal switch. Our structure consists of two carbon nanotubes as reservoirs linked by an azobenzene molecule. We use density functional tight binding method combined with atomistic Green’s functions to calculate the thermal conductance. We show that thermal conductance can be altered significantly by switching the molecule from trans to cis configuration and vice versa. We further investigate the performance of the thermal switch by using different molecules and linkers.

Please indicate your preference:

Poster Presentation: [x]

Molecular dynamics simulations study of temperature effect on phonon dispersion of two dimensional materials

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Many properties of crystalline materials such as thermal expansion and thermal conductivity are related to the phonon density of states and phonon spectrum. So far, many other properties of two dimensional materials have been determined accurately by ab-initio simulations. However, first principle calculations based on density functional theory for determining phonon dispersion suffer from the fact they work only at zero temperature. We presented a systematic study of phonon properties of some two dimensional materials at finite temperature by using atomic trajectories and velocities extracted from molecular dynamics simulations which take into account all anharmonic effects.

<u>Please indicate your preference:</u>

Poster Presentation: [X**]**

Width Independent Nanoribbons of TiS_3

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There are a few theoretical investigations on the electronic properties of two-dimensional TiS_3 [1,2], characteristic properties of one-dimensional nanoscale structures of TiS_3 nanoribbons (TiS_3NRs) have not been explored. Therefore, we investigate the electronic properties, mobility and strain response of TiS_3NRs from first-principles calculations.[3] Two types of ribbons with different orientations are studied, labeled as **a-** TiS_3NRs and **b-** TiS_3NRs. The **a-** TiS_3NRs have large edge energy ranging from 450 to 480 meV/A^0. On the other hand, the **b**-TiS_3NRs are found to have small edge energy around 60 meV/ A^0, suggesting that their isolation from 2D monolayer is not difficult. All the **a-** TiS_3NRs metallic, and exhibit non-zero magnetic moment. The spin density is contributed mostly by edge atoms. On the contrast, all the **b-** TiS_3NRs have direct band gaps at the Gamma point. Interestingly, the gap value and the band edge position are almost independent of the ribbon width, indicating strong edge effects. This feature promises a constant band gap in a **b**-TiS_3NRs with rough edge, where the ribbon width differs in different regions. The bandgap and the band edge position of **b**-TiS_3NRs are quite sensitive to applied strain. It increases with increasing tensile strain, and a direct-to-indirect band gap transition can be triggered by strain. In addition, we investigate the termination of ribbon edges by hydrogen atoms. Upon edge passivation, the metallic and magnetic features of **a**-TiS_3NRs remain unchanged, while the band gap of **b**-TiS_3NRs is increased significantly. The robust metallic and ferromagnetic nature of **a**-TiS_3NRs is an essential feature for spintronic device applications. The direct, width-independent and strain tunable bandgap of **b**-TiS_3NRs is potential importance in many fields of nanoelectronics, such as field-effect devices, opto-electronic applications and strain sensor.

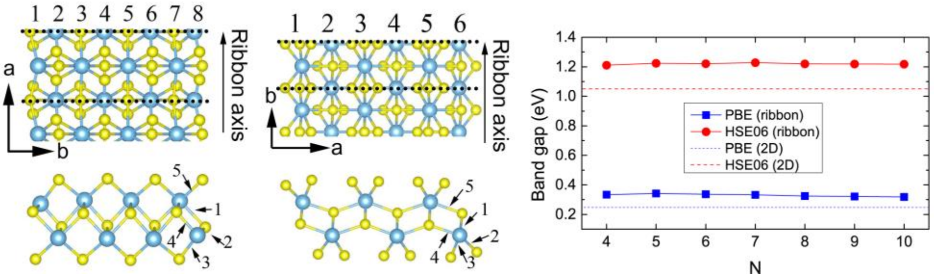

Fig 1. Top and side view of an 8-**a**-TiS_3NR and 6-**b**-TiS_3NR. a and b are the lattice vectors of the 2D TiS_3. The bandgap as a function of the **b**-TiS_3NR width *N*. Both GGA-PBE and HSE06 results are given. The dashed lines are the values for the 2D case.

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Acknowledgments:Computational resources were provided by TUBITAK ULAKBIM, High Performance and Grid Computing Center (TR-Grid e-Infrastructure). H.D.O., H.S., and R.T.S. acknowledge the support from TUBITAK Project No 114F397.

Poster Presentation: [x]

1T phase of TMDs Nanoribbon: $TiSe_2$

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Despite the comprehensive research on graphene and layered TMDs, studies on the electronic properties of T phase TMDs are sparse. Very recently, Peng *et al.* grew 1T-$TiSe_2$ ultrathin films on a graphitized SiC(0001) substrate by using molecular beam epitaxy.[1] Apart from this study, very recently synthesized $TiSe_2$ is a widely studied two-dimensional TMD [2,3] and has interesting properties. Motivated by the successful molecular beam epitaxy growth of $TiSe_2$ ultrathin films down to monolayer thickness, we investigate the one-dimensional nanoscale structures of $TiSe_2$ nanoribbons [4] because of its interesting electronic and physical properties that are essentially related with low dimensionality. The fully optimized NRs exhibit structural deviation at the edges. Especially for armchair ribbons are strongly distorted after relaxation, compared to zigzag ribbons. At the edges the Ti -Se bond lengths decrease because of the irregular force on the edge atoms. Nevertheless, the triple-layer networks are well kept intact for ribbons. The electronic band dispersion of $TiSe_2$ NRs show similar behavior like the monolayer $TiSe_2$. The electronic band gap of the nanoribbons decreases exponentially with the width and vanishes for ribbons wider than 20 A^0. For ultranarrow zigzag-edged nanoribbons we find odd-even oscillations in the band gap width, although their band structures show similar features. In fact, we found that reducing dimensionality from 2D to 1D, at a certain ribbon width a metal to semiconductor transition is found for both type of ribbons.

In addition, the robust metallic behavior of both zigzag and armchair $TiSe_2$ NRs remains unaltered even after passivation of the edges by hydrogen atoms. Moreover, our calculations demonstrates that $TiSe_2$ NRs are not magnetic and the edge states do not effect the magnetization of the structures. Our results shed light on the characteristic properties of T phase nanoribbons of similar crystal structures.

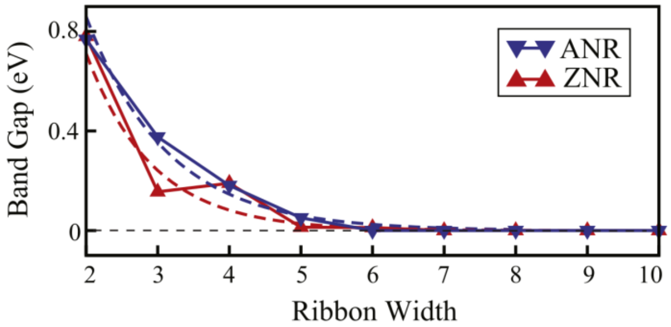

Fig 1. Energy gap of zigzag ($2 \leq N_z \leq 10$) and armchair ($2 \leq N_a \leq 10$) 1T-$TiSe_2$ nanoribbons as function of the ribbon width. Dashed curves are exponential fits.

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Acknowledgments: Computational resources were provided by TUBITAK ULAKBIM, High Performance and Grid Computing Center (TR-Grid e-Infrastructure). H.D.O., H.S., and R.T.S. acknowledge the support from TUBITAK Project No 114F397.

Poster Presentation: [x]

Platinum clusters on Graphene, 1H-MoS$_2$ and 1T-TaS$_2$

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Many experiments and theoretical studies have revealed that the surfaces of graphene and graphene-like structures can play an active role as a host surface for clusterization of transition metal atoms [1,2]. Motivated by these observations, we investigate theoretically the adsorption, diffusion and magnetic properties of Pt clusters on three different two-dimensional atomic crystals using first principles density functional theory.[3] We found that monolayers of graphene, molybdenum disulfide (1H-MoS2) and tantalum disulfide (1T-TaS2) provide different nucleation characteristics for Pt cluster formation. At low temperatures, while the bridge site is the most favorable site where the growth of a Pt cluster starts on graphene, top-Mo and top-Ta sites are preferred on 1H-MoS$_2$ and 1T-TaS$_2$, respectively. Ground state structures and magnetic properties of Pt$_n$ clusters (n = 2,3,4) on three different monolayer crystal structures are obtained. We found that the formation of Pt$_2$ dimer and a triangle-shaped Pt$_3$ cluster perpendicular to the surface are favored over the three different surfaces. While bent rhombus shaped Pt$_4$ is formed on graphene, the formation of tetrahedral shaped clusters are more favorable on 1H-MoS$_2$ and 1T-TaS$_2$. Our study of the formation of Pt$_n$ clusters on three different monolayers provides a gateway for further exploration of nanocluster formations on various surfaces.

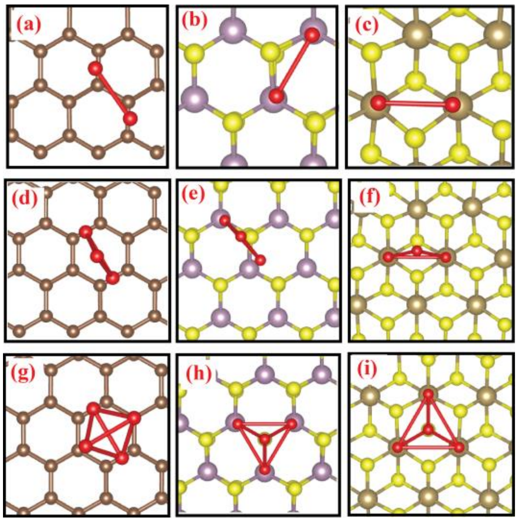

Fig 1. Most stable configurations for Pt$_n$-clusters on three different substrates, graphene (left column), MoS$_2$ (middle column) and TaS$_2$ (right column). The red balls denote Pt atoms.

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Acknowledgments: Computational resources were provided by TUBITAK ULAKBIM, High Performance and Grid Computing Center (TR-Grid e-Infrastructure). H.D.O., H.S., and R.T.S. acknowledge the support from TUBITAK Project No 114F397.

Poster Presentation: [x]

Graphene growth by Inductively-Coupled Plasma Chemical Vapor Deposition at Low Temperature

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The outstanding electrical, mechanical, optical and thermal properties of graphene, resulted in tremendous interest on this material for potential applications that include touch screens, light emitting diodes and printed electronics.[1-3] Several recent studies showed that a highly promising approach to grow graphene at reduced temperatures and processing times is to use plasma enhanced CVD (PECVD). Here the excitement of the reactant gases by the plasma lowers the activation energy for the growth of graphene and provides a low temperature route. The previous studies used PECVD systems that rely on surface wave plasma,[4] microwave plasma,[5] plasma assisted thermal CVD,[6] inductively coupled plasma CVD,[7, 8] and pulsed DC plasma reactor[11] to synthesize graphene at temperatures between 300 °C to 950 °C. This study for the growth of graphene at a low temperature of 300 °C using an inductively-coupled plasma chemical vapor deposition system. The results indicate bilayer graphene films with an intensity ratio (I_{2D}/I_G) of 2D band to G that equals to 1.1 and a thickness of 0.68 nm grown at low flow rates of CH_4 and low plasma powers for depositions as short as 20 s.

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Poster Presentation: [x]

Highly Efficient Graphene Supports for Fuel Cells

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Graphene nanomaterials are important because of their distinct properties such as high electrical conductivity, surface area and enormous stability. Therefore, graphene has been used as promising catalyst support in energy conversion and storage systems. In order to achieve high catalytic activity a specifically guided growth of catalyst on graphene support surface with delicate controllability is highly preferred. Therefore, we modify graphene surface in two different ways such as graphene functionalization with various active functional groups and fabrication of nanocomposites with intrinsically conducting polymers e.g. polypyrrole (PPy). We have successfully modified graphene oxide by the functionalization with free amine groups (GO-NH_2), RGD peptide (GO-RGD) and Nitrogen doping (N-GO). Platinum (Pt) catalyst nanoparticles are deposited on these functionalized GO (f-GO) using ethylene glycol modified method. The dispersion of Pt deposited F-GO has been enhanced and stable optimized dispersions in organic solvents were obtained. The cyclic voltametry (CV) results showed a high electrochemical surface area (ECSA) of 147 m^2/g for GO-RGD compared to Pt/carbon black (Pt/C, 80 m^2/g_{Pt}) and Pt/GO (99 m^2/g_{Pt}). On the other hand, we also fabricated GO/PPy/CB (carbon black) hybrid nanocomposites as catalyst support and deposited Pt catalyst nanoparticles. The CV results showed a high ECSA of 153 m^2/g_{Pt}. These modified graphene nanomaterials including Pt/f-GO and hybrid composites have been successfully used in proton exchange membrane fuel cell (PEMFC) electrodes. The Pt nanoparticles distribution on various modified graphene surfaces, which may significantly influence their properties such as electrical conductivity, electrocatalytic activity when they used as catalyst support and fuel cell performance will be discussed more in details.

Please indicate your preference:

Oral Presentation: [ ]

Poster Presentation: [x]

Superlubricity and Frictional Force of Bilayer Graphene System

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In recent years, extensive work on friction of surfaces at atomistic scale lead to well developed research area called nano-tribology. The connection from atomistic scale to macroscopic friction is mainly done using molecular dynamics methods [1]. However, the required atomistic potentials for the molecular dynamics calculations needs to be extracted from ab initio calculations [2]. Moreover, the atomistic properties are also important in order to understand detailed processes from stick-slip to energy dissipation occurred during frictional force microscopy experiments, especially on different types of two dimensional materials (graphene, MoS_2, h-BN, WS_2). The interpretation of the nano friction experiments needs more expressive models rather than basic Tomlinson model [3]. Also, to this end, atomistic calculations would be crucial to employ. In this study, the frictional force between two graphene surfaces has been investigated by using first-principles calculations based on density functional theory. We considered six different geometric configurations, such as bilayer graphene (perfect), B-doped graphene/graphene, N-doped graphene/graphene, single vacancy defected graphene/graphene, double vacancy defected graphene/graphene, and graphane/graphene surfaces. On our calculations, one graphene layer (perfect, doped, with vacancy defect, graphane) has been moved relative to perfect graphene surface. Eventually, the binding energy, interlayer distance, frictional force and orbital nature of actual interactions are explored after the optimized geometries.

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This work is supported by TUBITAK Project No: 114F162

Please indicate your preference:

Poster Presentation: [X]

Mechanical Behaviors of Two-Dimensional Transition Metal Dichalcogenide Bilayers

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Lamellar transition-metal dichalcogenides (TMDCs) whose layers are held together by van der Waals forces have attracted considerable interest for potential applications ranging from nano-electronics to nano-tribology especially due to their lubricating behavior. We investigated the sliding mechanisms of TMDC bilayers of the type MX_2, with M transition metal atom (Mo, W.) and X chalcogen atom (S, Se, or Te.), including heterostructures of MX_2 by means of quantum mechanical first principles calculations based on density functional theory including van der Waals dispersion. Friction properties of those homo- and hetero- bilayers of MX_2 are studied by performing friction force calculation under different load and environment (like defects, ad-atoms etc.) conditions. Based on the results, we provide an understanding of tuning the friction on nanoscale.

Please indicate your preference:

Poster Presentation: [x]

Synthesis and Functionalization of Large Area CVD Graphene with Cu Nanoparticles for Biosensor

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Since its discovery in 2004, graphene is dedicated as a wonder material that exhibits excellent mechanical, electrical, thermal, tribological and optical properties thereby it has potential usage in numerous applications such as electronic devices, supercapacitors, lubricants, composite materials, flexible transparent displays and sensors [1,2]. To date many methods have been studied to obtain high quality monolayer graphene in large scale and among them the most promising technique is chemical vapor deposition (CVD) method, in particular thermal CVD. Widely used CVD method are able to synthesize high-quality graphene on transition metals, such as nickel or copper, in the presence of a carbon supply as hydrocarbons or alcohols [3].

Functionalization of graphene with nanoparticles which induces new properties to graphene will increase its area of utilization in materials science, graphene based instruments and sensors [4]. Decorating graphene with Cu nanoparticles promises to detect of glucose in the blood. Since Cu nanoparticles are generally is produced by reducing and capping agents via chemical process, production is not be as desired.

In this study, we have developed a new approach for synthesis of Cu NPs/graphene to use in biosensor applications. Firstly large area graphene (2x2 cm^2) was prepared by CVD on the Cu foils and transferred onto SiO_2 substrates by transfer process. As the optimal parameters for Cu nanoparticles defined to decorate graphene samples, nanoparticles were collected on graphene/SiO_2 by magnetron sputtering technique.

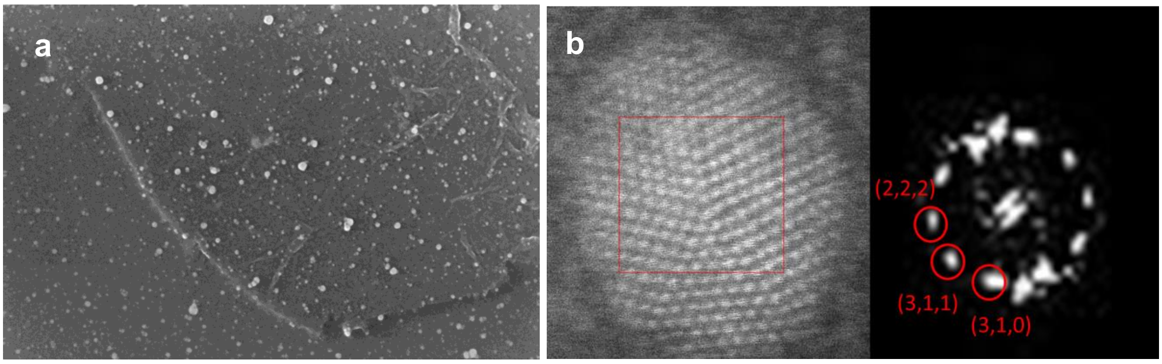

Figure: a) SEM picture of Cu nanoparticles on graphene **b)** HRTEM analysis of Cubic Cu nanoparticle.

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Poster Presentation: [X]

Group V Monolayer Holey Graphene Crystals

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Motivated by a recent experiment that reported the synthesis of a new 2D material nitrogenated holey graphene (C_2N) [Mahmood *et al.,* Nat. Comm., 2015, 6, 6486], electronic, magnetic, and mechanical properties of nitrogenated (C_2N), phosphorated (C_2P) and arsenicated (C_2As) monolayer holey graphene structures are investigated using first-principles calculations[1]. Our total energy calculations indicate that, similar to the C_2N monolayer, the formation of the other two holey structures are also energetically feasible. Calculated cohesive energies for each monolayer show a decreasing trend going from C_2N to C_2As structure. Remarkably, the holey monolayers with N and As are direct band gap semiconductors, while the one with P is an indirect-gap semiconductor. Regarding the mechanical properties (in-plane stiffness and Poisson ratio), we find that C_2N has the highest in-plane stiffness and the largest Poisson ratio among the three monolayers. In addition, our calculations reveal that for the C_2N, C_2P and C_2As monolayers, creation of N and P defects changes the semiconducting behavior to a metallic ground state while the inclusion of double H impurities in all holey structures results in magnetic ground states. As an alternative to the experimentally synthesized C_2N, C_2P and C_2As are mechanically stable and flexible semiconductors which are important for potential applications in optoelectronics.

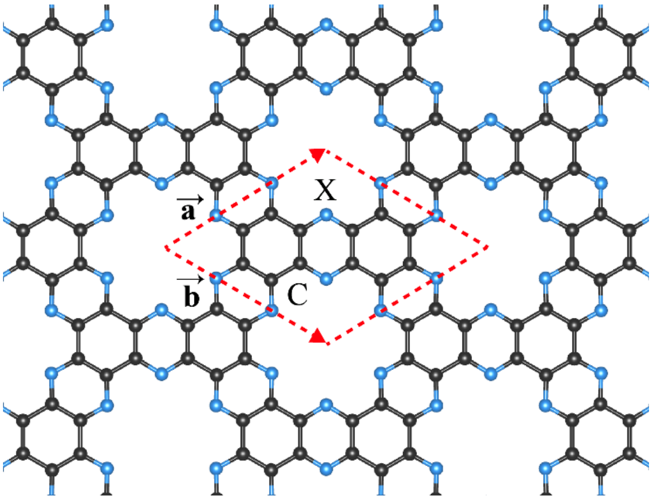

Figure: Top view of C_2X holey graphene monolayer structure where X represents N, P or As atoms.

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<u>Please indicate your preference:</u>

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Poster Presentation: [x]

Electric Field Driven Bandgap Crossover in $Mg(OH)_2$-WS_2 Heterobilayer

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Magnesium hydroxide ($Mg(OH)_2$) has a layered brucite-like structure in its bulk form and was recently isolated as a new member of 2D monolayer materials. We investigated the electronic and optical properties of monolayer crystals of $Mg(OH)_2$ and WS_2 and their possible heterobilayer structure by means of first principles calculations. It was found that both monolayers of $Mg(OH)_2$ and WS_2 are direct-gap semiconductors and these two monolayers form a typical van der Waals heterostructure with a weak interlayer interaction and a type-II band alignment with a staggered gap that spatially separates electrons and holes. We also showed that an out-of-plane electric field induces a transition from a staggered to a straddling type heterojunction. Moreover, by solving the Bethe-Salpeter equation on top of single shot G_0W_0 calculations, we show that the oscillator strength of the intralayer excitons of the heterostructure is an order of magnitude larger than the oscillator strength of the interlayer excitons which is an expected result since the electrons and the holes of the interlayer excitons are weakly coupled electronically. Because of the staggered interfacial gap and the field-tunable energy band structure, the $Mg(OH)_2$ - WS_2 heterobilayer can become an important candidate for various optoelectronic device applications in nanoscale.

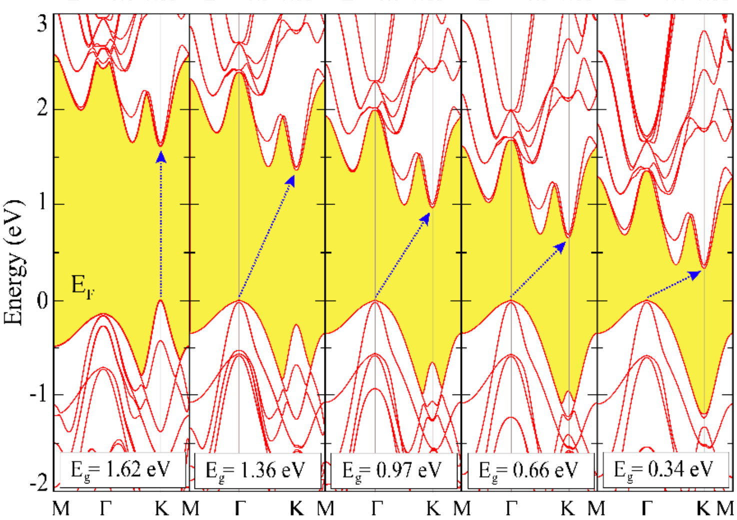

Figure: The effect of an external out-of-plane electric field on the band structure of the heterobilayer. The band gap regions are highlighted in yellow.

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Please indicate your preference:

Oral Presentation: [ ]

Poster Presentation: [x]

Electronic and Mechanical Properties of Pentagonal Monolayer Crystals

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In the last decade, graphene has become one of the most exciting topics of materials research due to its exceptional properties. Recently a new form of C atoms, namely penta-graphene, has been proposed by Zhang *et al.* [1] In this study[2] we present a theoretical investigation of structural, electronic and mechanical properties of pentagonal monolayers of carbon (p-graphene), boron nitride (p-B_2N_4 and p-B_4N_2) and silver azide (p-AgN_3) by performing state-of-the-art first principles calculations. Our total energy calculations suggest feasible formation of monolayer crystal structures composed entirely of pentagons. In addition, electronic band dispersion calculations indicate that while p-graphene and p-AgN3 are semiconductors with indirect bandgaps, p-BN structures display metallic behavior. We also investigate the mechanical properties (in-plane stiffness and the Poisson's ratio) of four different pentagonal structures under uniaxial strain. p-graphene is found to have the highest stiffness value and the corresponding Poisson's ratio is found to be negative. Similarly, p-B_2N_4 and p-B_4N_2 have negative Poisson's ratio values. On the other hand, the p-AgN_3 has a large and positive Poisson's ratio. In dynamical stability tests based on calculated phonon spectra of these pentagonal monolayers, we found that only p-graphene and p-B_2N_4 are stable, but p-AgN_3 and p-B_4N_2 are vulnerable against vibrational excitations.

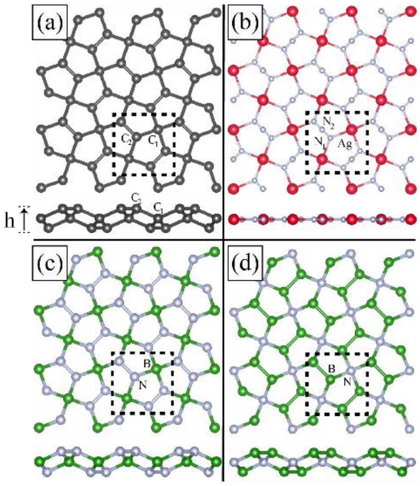

Figure: Top view and side view of pentagonal (a) graphene (b) AgN_3, (c) B_2N_4, (d) B_4N_2.

[1] S. Zhanga, J. Zhouc, Q. Wanga, X. Chend, Y. Kawazoef, P. Jenac, PNAS **112**, 2372 (2015).
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Please indicate your preference:

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Doping of Graphene by Nitrogen Plasma

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A significant advance toward achieving practical applications of graphene as a two-dimensional material would be provided by successful doping of both n-type and p-type. In addition, controllable carrier transport in due to charged impurities (donors or acceptors) in the graphene lattice is still lacking. Recently, it was shown nitrogen doping of graphene lattice can lead to a change in the carrier concentration and open a bandgap due to symmetry breaking [1]. Furthermore this was an effective way to customise the properties of graphene and exploit its potential for various application [2]. Here, we doped graphene with nitrogen by using a nitrogen plasma.

In this study, we grew large area graphene with methane and ethylene on copper foil at low pressure CVD. After the growth, the graphene films were transferred onto Si/SiO_2 and Au(200 nm)/mica substrate then samples were doped in a plasma chamber. The chamber pressure was reduced down to ~30mTorr in 5 min. After the placement of the transferred graphene into the chamber, the high purity N_2 (99.999%) with a flow of 4.1 - 23.1 sccm was regulated by a bleeding valve to set the chamber pressure in the range of 826 - 1060mTorr. Then N_2 was introduced into the chamber to create plasma by applying a radio-frequency forward power of 7 Watt (low power), 10 Watt (medium power) and 30 Watt (high power). Lastly, the plasma doping duration was varied between 5 and 20 min.s

We used Raman spectroscopy, scanning tunneling microscopy (STM) and Fourier transform infrared spectroscopy (FTIR) to characterize Nitrogen doped graphene (N-graphene). We also provide Raman mapping of N-graphene to show homogeneity of nitrogen doping in the graphitic lattice.

* This work was supported by TUBITAK Project number 112T946.

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Investigation of Tribological Properties of Metal Surface Coated with Monolayer Graphene

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Friction that has very important role in many areas of life is considered to be a major problem in the mechanical assembly due to leading wear of components. In order to prevent the decrease of working life and performance as a result of friction of materials that interact with other materials, friction and wear mechanism should be taken under control. Reducing friction in studies achieved by lubricating the contacting surfaces and lubricants were used in liquid and solid form. As a studied material for a long time graphite demonstrates very good lubricating properties. The single layer of graphite, graphene, occurred sp^2-bonded carbon atoms arranged in a honeycomb lattice, has attracted a plethora of attention because of its tribological properties as well as remarkable physical, electrical and optical properties. In the light of this information, monolayer graphene were grown on copper foils by CVD process and transferred onto metallic surface (journal bearing) to determine tribological behaviors. Structural analysis of the steel surface coated with graphene, were examined by optical microscopy and Raman spectroscopy, friction and wear characteristics were investigated by using of atomic force microscopy (AFM).

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Binding and Diffusion of Au and Ag atoms on few-layer graphyne

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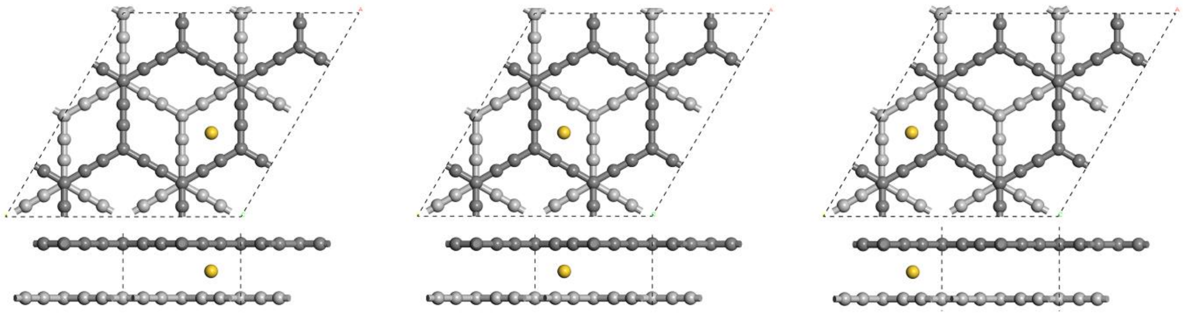
Up to now, diverse forms of carbon allotropes, such as fullerene, nanotubes, graphene have been successfully synthesized. These progresses have promoted rapid development of material science and nanotechnology. Graphyne, analog to graphene, possesses remarkable properties, such as small carrier effective mass, advanced hydrogen storage capacity, and high carrier mobility at room temperature [1-6].

In this study, we performed first-principles calculations with density functional theory (DFT) implemented in the Vienna Ab Initio Simulation Package (VASP) [7]. First of all, we have investigated the structure of α-graphyne in its bilayer form. As bilayer graphene, it exhibits for different stacking modes. The most stable stacking mode for α-graphyne is AB stacking in few other reports [8]. It was studied the structural properties, such as lattice parameter and the interlayer distance, for this stacking mode. Secondly, we have calculated the adsorption energies, preferred binding sites, equilibrium distances, and preferred diffusion paths for structure of Ag_{1-3} and Au_{1-3} on mono- and bi-layer graphyne. And finally, we discuss the initial clustering process of silver and gold on bilayer graphyne. For instance; we simulated the formation of a dimer out of two pre-adsorbed Ag (or Au) atoms. At the same time, the formation of a trimer out of a dimer and adatom was studied.



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Graphene-Atmosphere Interactions: Response to Pressure, Temperature and Humidity

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Since the early days of its first isolation, the detection of gas molecules as well as humidity and temperature by use of graphene have been a matter of interest [1]. We have used graphene crystals grown by ambient chemical vapor deposition (AP-CVD) to produce graphene based sensors. We employed a homemade atmospheric control chamber in order to investigate the response of the resistivity of the graphene films to pressure, temperature and humidity changes. Under constant voltage, the resistance of the graphene samples was observed to change as a function of humidity and resistance of the films showed a response very similar to the humidity values given by a high precision commercial humidity sensor. Interestingly we observed decrease of the resistivity on graphene device as a function of increasing humidity on several samples in contrast to earlier reports [2].

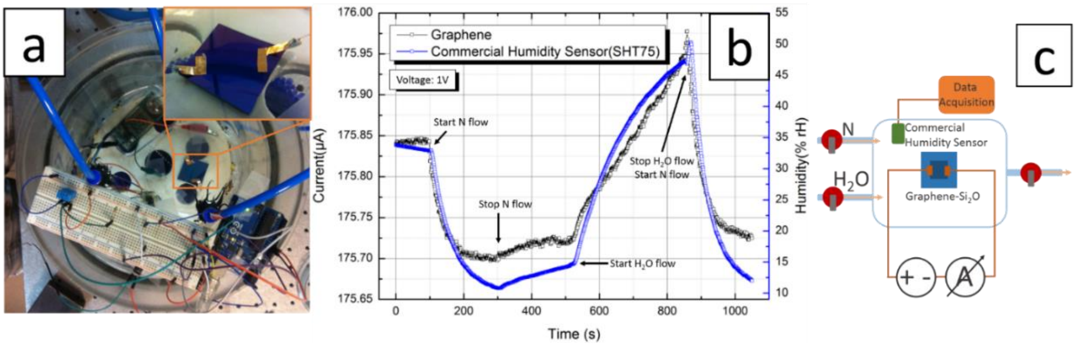

Figure: a) A photograph of the setup, inset the Graphene-Si$_2$O device. b) Response of the commercial humidity sensor and the graphene device to different humidity levels. c) A depiction of the experimental setup.

In this presentation the response of the resistivity of graphene to several atmospheric conditions will be shown and the effect of water films on the resistivity of graphene will be discussed.

This work was supported by TÜBİTAK-1003 project with grant number 114F036.

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Optically Visible Epitaxial Graphene Ridges on SiC Substrates

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Superior physical, optical and electronic properties of graphene has placed this extraordinary material to the spotlight of many research groups around the world by means of either a deeper understanding of its properties or the possible applications for various technological devices. Among a variety of techniques developed to produce this single-atom thick material, epitaxial growth method stands out for acquiring impressively large-scale and uniform graphene layers. Regardless of the growth techniques, structural defects of the honey-comb lattice of graphene such as vacancies, grain boundaries, pentagon-heptagon defects, and out-of- plane deformations are still present in the graphene matrix. In the case of graphene growth on SiC substrate, the lattice mismatch between epitaxial graphene and silicon carbide gives rise to a strong compressive strain and hence leads to the formation of ridges, ripples and folds on the graphene layer.

In our work, single layer epitaxial graphene template with great thickness uniformity was grown on a SiC semiconducting substrate by using high temperature ultra-high vacuum annealing process. We found that hexagon shaped wrinkles became visible only after coating a thin layer of SiO_x on epitaxial graphene. The wrinkle formation on epitaxial graphene were characterized by using optical microscopy, scanning electron microscopy and atomic force microscopy measurements as shown in the figures.

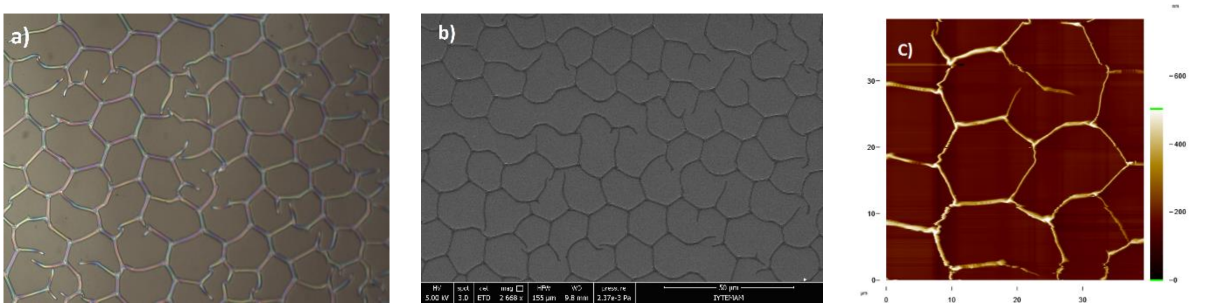

Figure a) Optical microscopy image of epitaxial graphene ridges b) SEM image of epitaxial graphene ridges c) AFM image of epitaxial graphene image

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Measurement Artifacts in High-Resolution Scanning Probe Microscopy Due to Probe Effects

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Scanning probe microscopy (SPM) is a family of powerful experimental tools that can be used, for instance, to (i) measure atomic-scale force fields on samples surfaces (via atomic force microscopy, AFM) and (ii) measure electronic properties of sample surfaces with atomic specifity (via scanning tunneling microscopy, STM). Consequently, physical interpretation of high-resolution SPM data and the determination of potential measurement artifacts are of great significance. In this work, we focus on two different sources that may cause measurement artifacts in high-resolution SPM experiments: tip stiffness and tip asymmetry. In particular, we perform numerical simulations of SPM experiments on the ionic crystal surface of NaCl (100) and a two-layer graphene sample, employing a model tip apex consisting of several Pt atoms in close-packed configuration and Lennard-Jones interactions [1, 2]. It is found that tip stiffness has a significant effect on the appearance of atomic-scale structural features in AFM images acquired on NaCl (100). Moreover, it is determined that tip asymmetry may also cause significant spatial distortion of atomic-scale features in both AFM and STM images, and at the same time, lead to erroneous interpretations of local chemical reactivity on graphene [2].

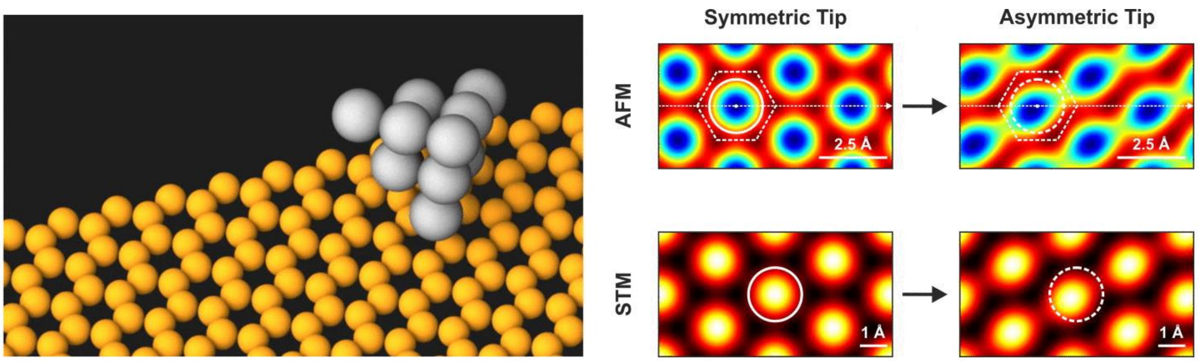

Figure: Model tip and sample surface employed in numerical simulations of the effect of tip asymmetry (left) and the effect of tip asymmetry on high-resolution AFM and STM imaging (right) [2].

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