Alex Kutana **March 2022**

CONTACT INFORMATION

Materials Science and NanoEngineering
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RESEARCH INTERESTS

My research focuses on theoretical studies of electronic, optical, mechanical, and thermodynamical properties of nanoscale and low-dimensional materials and computational materials design.

EMPLOYMENT

Research Scientist, Rice University (2016–current), Postdoctoral Scholar, Rice University (2012–2016), Naval Research Laboratory (2010–2012), University of Florida (2009–2010), California Institute of Technology (2003–2009)

TEACHING EXPERIENCE

- Teaching course (MSNE 433/533, Computational Materials Modeling) at Rice University

EDUCATION

Ph.D. in Chemistry (2003), University of Houston, Houston, TX

- Advisor: J. W. Rabalais
- Thesis: *Structure and gas adsorption kinetics for monocrystalline surfaces studied with low energy ion scattering*

B.S. in Radiophysics and Electronics (1996), Kiev National University, Kiev, Ukraine

- Diploma with honors

PUBLICATIONS

1. Henry Yu, Alex Kutana, and Boris I. Yakobson. Electron Optics and Valley Hall Effect of Undulated Graphene *Nano Letters* , (2022).

2. Qin-Kun Li, Alex Kutana, Evgeni S. Penev, and Boris I. Yakobson. Iron corrosion in the "inert" supercritical CO2, ab initio dynamics insights: How impurities matter *Matter* **5**, 1–12 (2022).

3. Alex Kutana, Tariq Altalhi, Qiyuan Ruan, Jun-Jie Zhang, Evgeni S. Penev, and Boris I. Yakobson. Stability and electronic properties of gallenene *Nanoscale Advances* , (2022).

4. Evgeni S. Penev, Yuanyue Liu, Tariq Altalhi, Alex Kutana, and Boris I. Yakobson. Stable Low-Dimensional Boron Chalcogenides from Planar Structural Motifs *Journal of Physical Chemistry A* **125**, 6059–6063 (2021).

5. Seyed Mohammad Sajadi, Shayan Enayat, Lívia Vásárhelyi, Alessandro Alabastri, Minghe Lou, Lucas M. Sassi, Alex Kutana, Sanjit Bhowmick, Christian Durante, Ákos Kukovecz, Anand B. Puthirath, Zoltán Kónya, Robert Vajtai,

Peter Boul, Chandra Sekhar Tiwary, Muhammad M. Rahman, and Pulickel M. Ajayan. Three-dimensional Printing of Complex Graphite Structures *Carbon* **181**, 260–269 (2021).

6. Henry Yu, Sunny Gupta, Alex Kutana, and Boris I. Yakobson. Dimensionality-Reduced Fermi Level Pinning in Coplanar 2D Heterojunctions *The Journal of Physical Chemistry Letters* **12**, 4299–4305 (2021).

7. Govind Chilkoor, Namita Shrestha, Alex Kutana, Manoj Tripathi, Francisco C. Robles Hernandez, Boris I. Yakobson, Meyya Meyyappan, Alan B. Dalton, Pulickel M. Ajayan, Muhammad M. Rahman, and Venkataramana Gadhamshetty. Atomic Layers of Graphene for Microbial Corrosion Prevention *ACS Nano* **15**, 447–454 (2020).

8. Govind Chilkoor, Kalimuthu Jawaharraj, Bhuvan Vemuri, Alex Kutana, Manoj Tripathi, Divya Kota, Taib Arif, Tobin Filleter, Alan B. Dalton, Boris I. Yakobson, M. Meyyappan, Muhammad M. Rahman, Pulickel M. Ajayan, and Venkataramana Gadhamshetty. Hexagonal Boron Nitride for Sulfur Corrosion Inhibition *ACS Nano* **14**, 14809–14819 (2020).

9. Sunny Gupta, Alex Kutana, and Boris I. Yakobson. Heterobilayers of 2D materials as a platform for excitonic superfluidity *Nature Communications* **11**, 2989, 1–7 (2020).

10. Vasilii I. Artyukhov, Sunny Gupta, Alex Kutana, and Boris I. Yakobson. Flexoelectricity and charge separation in carbon nanotubes *Nano Letters* **20**, 3240–3246 (2020).

11. Yosuke Uchiyama, Alex Kutana, Kenji Watanabe, Takashi Taniguchi, Kana Kojima, Takahiko Endo, Yasumitsu Miyata, Hisanori Shinohara, and Ryo Kitaura. Momentum-forbidden dark excitons in hBN-encapsulated monolayer MoS2 *npj 2D Materials and Applications* **3**, 26, 1–6 (2019).

12. Sunny Gupta, Sharmila N. Shirodkar, Alex Kutana, and Boris I. Yakobson. In Pursuit of 2D Materials for Maximum Optical Response *ACS Nano* **12**, 10880–10889 (2018).

13. Sandhya Susarla, Jordan A. Hachtel, Xiting Yang, Alex Kutana, Amey Apte, Zehua Jin, Robert Vajtai, Juan Carlos Idrobo, Jun Lou, Boris I. Yakobson, Chandra Sekhar Tiwary, and Pulickel M. Ajayan. Thermally Induced 2D Alloy-Heterostructure Transformation in Quaternary Alloys *Advanced Materials* **30**, 1870344, 1–6 (2018).

14. Sunny Gupta, Alex Kutana, and Boris I. Yakobson. Dirac Cones and Nodal Line in Borophene *The Journal of Physical Chemistry Letters* **9**, 2757–2762 (2018).

15. Mitsuhiro Okada, Alex Kutana, Yusuke Kureishi, Yu Kobayashi, Yuika Saito, Tetsuki Saito, Kenji Watanabe, Takashi Taniguchi, Sunny Gupta, Yasumitsu Miyata, Boris I. Yakobson, Hisanori Shinohara, and Ryo Kitaura. Direct and Indirect Interlayer Excitons in a van der Waals Heterostructure of hBN/WS2/MoS2/hBN *ACS Nano* **12**, 2498–2505 (2018).

16. Sandhya Susarla, Vidya Kochat, Alex Kutana, Jordan A. Hachtel, Juan Carlos Idrobo, Robert Vajtai, Boris I. Yakobson, Chandra Sekhar Tiwary, and Pulickel M. Ajayan. Phase Segregation Behavior of 2D Transition Metal Dichalcogenide Binary Alloys Induced by Dissimilar Substitution *Chemistry of Materials* **29**, 7431–7439 (2017).

17. Sandhya Susarla, Alex Kutana, Jordan A. Hachtel, Vidya Kochat, Amey Apte, Robert Vajtai, Juan Carlos Idrobo, Boris I. Yakobson, Chandra Sekhar Tiwary, and Pulickel M. Ajayan. Quaternary 2D Transition Metal Dichalcogenides (TMDs) with Tunable Bandgap *Advanced Materials* **29**, 1702457, 1–8 (2017).

18. Jincheng Lei, Alex Kutana, and Boris I. Yakobson. Predicting Stable Phase Monolayer Mo2C (MXene), a Superconductor with Chemically-Tunable Critical Temperature *Journal of Materials Chemistry C* **5**, 3438–3444 (2017).

19. Ziang Zhang, Alex Kutana, Ajit Roy, and Boris I. Yakobson. NanoChimneys: Topology and Thermal Conductance of 3D Nanotube-Graphene Cone Junctions *The Journal of Physical Chemistry C* **121**, 1257–1262 (2017).

20. Ziang Zhang, Alex Kutana, Yang Yang, Nina V. Krainyukova, Evgeni S. Penev, and Boris I. Yakobson. Nanomechanics of carbon honeycomb cellular structures *Carbon* **113**, 26–32 (2017).

21. Henry Yu, Alex Kutana, and Boris I. Yakobson. Carrier Delocalization in Two-Dimensional Coplanar p-n Junctions of Graphene and Metal Dichalcogenides *Nano Letters* **16**, 5032–5036 (2016).

22. Zhiming Shi, Alex Kutana, Guangtao Yu, Wei Chen, Boris I. Yakobson, Udo Schwingenschlogl, and Xuri Huang. Tailoring the Electronic and Magnetic Properties of Two-Dimensional Silicon Carbide Sheets and Ribbons by Fluorination *The Journal of Physical Chemistry C* **120**, 15407–15414 (2016).

23. Evgeni S. Penev, Alex Kutana, and Boris I. Yakobson. Can two-dimensional boron superconduct? *Nano Letters* **16**, 2522–2526 (2016).

24. Alex Kutana, Andrii Goriachko, Zhili Hu, Hermann Sachdev, Herbert Over, and Boris I. Yakobson. Buckling Patterns of Graphene-Boron Nitride Alloy on Ru(0001) *Advanced Materials Interfaces* **2**, 1500322, 1–8 (2015).

25. Zhiming Shi, Zhuhua Zhang, Alex Kutana, and Boris I. Yakobson. Predicting Two Dimensional Silicon Carbide Monolayers *ACS Nano* **9**, 9802–9809 (2015).

26. Miao Zhang, Guoying Gao, Alex Kutana, Yanchao Wang, Xiaolong Zou, John S Tse, Boris I. Yakobson, Hongdong Li, Hanyu Liu, and Yanming Ma. Two-Dimensional Boron-Nitrogen-Carbon Monolayers with Tunable Direct Band Gaps *Nanoscale* **7**, 12023–12029 (2015).

27. Luqing Wang, Alex Kutana, Xiaolong Zou, and Boris I. Yakobson. Electro-Mechanical Anisotropy of Phosphorene *Nanoscale* **7**, 9746–9751 (2015).

28. Zhiming Shi, Alex Kutana, and Boris I. Yakobson. How Much N-Doping can Graphene Sustain? *The Journal of Physical Chemistry Letters* **6**, 106–112 (2015).

29. Ziang Zhang, Alex Kutana, and Boris I. Yakobson. Edge reconstruction-mediated graphene fracture *Nanoscale* **7**, 2716–2722 (2015).

30. Luqing Wang, Alex Kutana, and Boris I. Yakobson. Many-body and spin-orbit effects on direct-indirect band gap transition of strained monolayer MoS2 and WS2 *Annalen der Physik* **526**, L7–L12 (2014).

31. Mingjie Liu, Alex Kutana, Yuanyue Liu, and Boris I. Yakobson. First-Principles Studies of Li Nucleation on Graphene *The Journal of Physical Chemistry Letters* **5**, 1225–1229 (2014).

32. Alex Kutana, Evgeni S. Penev, and Boris I. Yakobson. Engineering electronic properties of layered transition-metal dichalcogenide compounds through alloying *Nanoscale* **6**, 5820–5825 (2014).

33. A.Kutana and S.C.Erwin. Nonpolar GaN films on high-index silicon: lattice matching by design *Physical Review B* **87**, 045314, 1–9 (2013).

34. A.Kutana and S.C.Erwin. PbSe nanocrystals remain intrinsic after surface adsorption of hydrazine *Physical Review B* **83**, 235419, 1–4 (2011).

35. A.Kutana and K.P.Giapis. First-Principles Study of Chemisorption of Oxygen and Aziridine on Graphitic Nanostructures *Journal of Physical Chemistry C* **113**, 14721–14726 (2009).

36. M.J.Gordon, X.D.Qin, A.Kutana, and K.P.Giapis. Gas-Surface Chemical Reactions at High Collision Energies? *Journal of the American Chemical Society* **131**, 1927–1930 (2009).

37. A.Kutana and K.P.Giapis. Analytical carbon-oxygen reactive potential *Journal of Chemical Physics* **128**, 234706, 1–8 (2008).

38. A.Kutana and K.P.Giapis. Contact angles, ordering, and solidification of liquid mercury in carbon nanotube cavities *Physical Review B* **76**, 195444, 1–5 (2007).

39. A.Kutana and K.P.Giapis. Transient deformation regime in bending of single-walled carbon nanotubes *Physical Review Letters* **97**, 245501, 1–4 (2006).

40. A.Kutana, K.P.Giapis, J.Y.Chen, and C.P.Collier. Amplitude response of single-wall carbon nanotube probes during tapping mode atomic force microscopy: Modeling and experiment *Nano Letters* **6**, 1669–1673 (2006).

41. A.Kutana, M.J.Gordon, and K.P.Giapis. Neutralization of hyperthermal Ne+ on metal surfaces *Nuclear Instruments & Methods In Physics Research Section B-beam Interactions With Materials and Atoms* **248**, 16–20 (2006).

42. A.Kutana and K.P.Giapis. Atomistic simulations of electrowetting in carbon nanotubes *Nano Letters* **6**, 656–661 (2006).

43. J.Y.Chen, A.Kutana, C.P.Collier, and K.P.Giapis. Electrowetting in carbon nanotubes *Science* **310**, 1480–1483 (2005).

44. P.A.W.Heide, C.Lupu, A.Kutana, and J.W.Rabalais. Factors affecting the retention of Cs+ primary ions in Si *Applied Surface Science* **231**, 90–93 (2004).

45. A.Kutana, T.Ito, I.L.Bolotin, B.Makarenko, and J.W.Rabalais. TOF-SARS study of hydrogen adsorption and desorption kinetics on Si(100) *Vacuum* **73**, 73–78 (2004).

46. A.Kutana, B.Makarenko, and J.W.Rabalais. Kinetics of H atom adsorption on Si(100) at 500-650 K *Journal of Chemical Physics* **119**, 11906–11911 (2003).

47. I.L.Bolotin, A.Kutana, B.N.Makarenko, and J.W.Rabalais. Scattering and recoiling mapping of the Kr-Pt(111) system by SARIS *Surface Science* **540**, 285–294 (2003).

48. A.Kutana, I.L.Bolotin, and J.W.Rabalais. Universal expression for blocking cone size based on the ZBL potential *Surface Science* **495**, 77–90 (2001).

49. A.Kutana, I.L.Bolotin, and J.W.Rabalais. Universal expression for blocking cone size in low energy ion scattering based on MD simulations *Computer Simulation Studies In Condensed-matter Physics XIV* **89**, 77–81 (2002).

50. I.L.Bolotin, A.Kutana, B.Makarenko, and J.W.Rabalais. Kinetics and structure of O-2 chemisorption on Ni(111) *Surface Science* **472**, 205–222 (2001).

51. K.M.Lui, I.Bolotin, A.Kutana, V.Bykov, W.M.Lau, and J.W.Rabalais. How do hydrogen atoms on surfaces affect the trajectories of heavier scattered atoms? *Journal of Chemical Physics* **111**, 11095–11100 (1999).

52. S.A.Bugaichuk, A.G.Kutana, and A.I.Khizhnyak. Spatial structure of holographic gratings in photorefractive crystals with a nonlocal response *Quantum Electronics* **27**, 727–731 (1997).

53. S.A.Bugaichuk, A.G.Kutana, A.I.Khizhnyak, and N.I.Tarashchenko. The dynamics of recording of a transmission grating during FWM in a photorefractive medium with nonlocal response *Ukrainian Journal of Physics* **42**, 678–683 (1997).

Invited and Contributed Talks and Posters

March 14, 2017, UNIST, ES16 Workshop, APS (American Physical Society) March 2015, APS March 2014, APS March 2013, APS March 2012, APS March 2011, ACS (American Chemical Society) Sept 2013, ACS Aug. 2012, ACS Aug. 2011, AVS (American Vacuum Society) Oct. 2007, AVS Nov. 2004, AVS Nov. 2003 meetings