

- CONTACT INFORMATION Materials Science and NanoEngineering
MS 325
Rice University
6100 Main St
Houston, TX 77005
phone: (713)348-5979
fax: (713)348-5423
kutana@rice.edu
<http://www.alexkutana.net/>
- 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 (1996), Kiev National University, Kiev, Ukraine
 - Diploma with honors
- PUBLICATIONS
1. 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).
 2. 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).
 3. 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).
 4. 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).

5. 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).
6. 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).
7. Zhiming Shi, Alex Kutana, Guangtao Yu, Wei Chen, Boris I. Yakobson, Udo Schwingenschogl, 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).
8. Evgeni S. Penev, Alex Kutana, and Boris I. Yakobson. **Can two-dimensional boron superconduct?** *Nano Letters* **16**, 2522–2526 (2016).
9. 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).
10. Zhiming Shi, Zhuhua Zhang, Alex Kutana, and Boris I. Yakobson. **Predicting Two Dimensional Silicon Carbide Monolayers** *ACS Nano* **9**, 9802–9809 (2015).
11. 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).
12. Luqing Wang, Alex Kutana, Xiaolong Zou, and Boris I. Yakobson. **Electro-Mechanical Anisotropy of Phosphorene** *Nanoscale* **7**, 9746–9751 (2015).
13. 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).
14. Ziang Zhang, Alex Kutana, and Boris I. Yakobson. **Edge reconstruction-mediated graphene fracture** *Nanoscale* **7**, 2716–2722 (2015).
15. 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).
16. 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).
17. 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).
18. 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).

19. A.Kutana and S.C.Erwin. **PbSe nanocrystals remain intrinsic after surface adsorption of hydrazine** *Physical Review B* **83**, 235419, 1–4 (2011).
20. 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).
21. 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).
22. A.Kutana and K.P.Giapis. **Analytical carbon-oxygen reactive potential** *Journal of Chemical Physics* **128**, 234706, 1–8 (2008).
23. 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).
24. A.Kutana and K.P.Giapis. **Transient deformation regime in bending of single-walled carbon nanotubes** *Physical Review Letters* **97**, 245501, 1–4 (2006).
25. 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).
26. 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).
27. A.Kutana and K.P.Giapis. **Atomistic simulations of electrowetting in carbon nanotubes** *Nano Letters* **6**, 656–661 (2006).
28. J.Y.Chen, A.Kutana, C.P.Collier, and K.P.Giapis. **Electrowetting in carbon nanotubes** *Science* **310**, 1480–1483 (2005).
29. 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).
30. 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).
31. 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).
32. 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).
33. 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).
34. 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).

35. 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).
36. 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).
37. 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).
38. 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