

Jing Yang

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3918 Pine Street, Apt. 3F, Philadelphia, PA 19104, USA

EDUCATIONS

- University of Pennsylvania, Philadelphia, Pennsylvania** **09/2012 ~ present**
- PhD candidate in physical chemistry
 - Advisor: Andrew M. Rappe
 - Expected graduation: 05/2018
- University of Waterloo, Waterloo, Ontario** **09/2010 ~ 08/2012**
- Master of Science in Chemistry (Nanotechnology)
 - Thesis title: *A study on para-hydrogen clusters at low temperature using centroid molecular dynamics*
- University of Waterloo, Waterloo, Ontario** **09/2007 ~ 06/2010**
- Bachelor of Science in Computational Science / Chemistry (Honours program)
 - Awards: Dean's honour's list for three consecutive years
- China University of Geosciences, Wuhan, China** **09/2005 ~ 07/2007**
- Bachelor of Engineering in Geographic Information System (GIS)

RESEARCH INTERESTS

- van der Waals interaction in molecular crystals
- Tribopolymer formation mechanism on micro- and nanomechanoelectrical devices
- First principle study of neutron scattering spectra of hybrid perovskites
- Pseudopotential development using hybrid density functionals

PROFESSIONAL SKILLS

- Programming: C, C++, Fortran, Python, Matlab
- Computational code development: Implement PBE0 hybrid density functional in OPIUM pseudopotential generator URL: <http://opium.sourceforge.net/>
- Computational Modeling: Quantum mechanics, Molecular dynamics
- Software: Abinit, FHI-AIMS, GAMESS, Gaussian, Quantum Espresso, Wannier90
- System Administrator: Maintaining local desktops, file server, and computation cluster of the research group
- Teaching Experience: Teaching Assistant for General Chemistry recitations in University of Pennsylvania (09/2012 ~ 05/2013, 09/2015 ~ 01/2016, 01/2017 ~ 05/2017)

PUBLICATIONS

- C. Ing, K. Hinsien, **J. Yang**, T. Zeng, H. Li, and P.-N. Roy, "A path-integral Langevin equation treatment of low-temperature doped helium clusters". *J. Chem. Phys.* 136, 224309 (2012)
- J. Tao, **J. Yang**, and A. M. Rappe, "Dynamical screening of van der Waals interactions in nanostructured solids: Sublimation of fullerenes". *J. Chem. Phys.* 142, 164302 (2015)
- F. Streller, G. E. Wabiszewski, D. B. Durham, F. Yang, **J. Yang**, Y. Qi, D. J. Srolovitz, A. M. Rappe,

and R. W. Carpick, “Novel Materials Solutions and Simulations for Nanoelectromechanical Switches”, IEEE Holm Conference on Electrical Contacts (Holm) 363-369 (2015)

- Y. Qi, **J. Yang**, and A. M. Rappe, “Theoretical Modeling of Tribochemical Reaction on Pt and Au Contacts: Mechanical Load and Catalysis”, ACS Appl. Mater. Interfaces, 8, 7529-7535 (2016)
- F. Streller, Y. Qi, **J. Yang**, F. Mangolini, A. M. Rappe, and R. W. Carpick, “Valence Band Control of Metal Silicide Films via Stoichiometry”, J. Phys. Chem. Lett., 7, 2573-2578 (2016)
- H. D. Kim, **J. Yang**, and A. M. Rappe, “Adsorption of Benzene on the RuO₂(110) Surface”, J. Phys. Chem. C, 121, 1585-1590 (2017)
- **J. Yang**, L. Z. Tan, and A. M. Rappe, “Hybrid functional pseudopotentials”, Phys. Rev. B 97, 085130 (2018)
- S. Sarkar, **J. Yang**, L. Z. Tan, A. M. Rappe, and L. Kronik, “Molecule-Adsorbed Topological Insulator and Metal Surfaces: a Comparative First Principles Study”, Chem. Mater., Just Accepted (S. Sarkar and **J. Yang** contributed equally to this work)
- **J. Yang**, Y. Qi, H. D. Kim, and A. M. Rappe, “Tribopolymer formation mechanism on the RuO₂ surface”, Phys. Rev. Appl. 9, 044038 (2018)

SELECTED CONFERENCE PROCEEDING

- June 5 ~ 9, 2011, the 94th Canadian Chemistry Conference and Exhibition, Montreal, QC
 - Theoretical and Physical Chemistry Session – Effective Potential Approach to the Simulation of Large Para-Hydrogen Clusters and Droplets (Oral)
- March 13 ~ 18, 2016, the 251st American Chemical Society National Meeting & Exposition Computers in Chemistry, San Diego, CA
 - Normal loading induced catalytic effect on tribopolymer formation on RuO₂(110) surface (Oral)
- March 23, 2016, the Catalysis Society of Metropolitan New York 2016 Annual Symposium, New Brunswick, NJ
 - Mechanical Stress Enhanced Tribopolymerization Mechanism of Metal and Metal Oxide Based Tiny Size Electromechanical Devices (Poster)
- March 13 ~ 17, 2017, APS March Meeting, New Orleans, LA
 - Hybrid density functional pseudopotentials (Oral)
- March 04 ~ 09, 2018, APS March Meeting, Los Angeles, CA
 - Oxidation and tribopolymerization mechanisms of Pt₃Si (001) surface (Oral)

AWARDS

- 2015 IEEE ERLE SHOBERT PRIZE PAPER AWARDEE
 - Novel Materials Solutions and Simulations for Nanoelectromechanical Switches
- 2018 Phase-I MolSSI Software Fellowships