LIQIU YANG

Contact: +86-18710207112 ‖*liqiuy@usc.edu*

EDUCATION

University of Southern California *2018 - 2023*
Ph.D., Chemical Engineering (Supervisor: Prof. Priya Vashishta)
Being invited to apply for the 2024 Viterbi Graduate Commencement Speaker *2024*

University of Chinese Academy of Sciences *2014 - 2018*
B.S., Chemistry
Excellent Graduate Award of Beijing *2018*
Excellent Graduate Award of University of Chinese Academy of Sciences *2018*

University of Southern California *2017 Fall*
Visiting Student for 1 semester

AWARDS AND HONORS

Being invited to apply for the 2024 Viterbi Graduate Commencement Speaker *2024*

Cover Image of JPCL (Vol 13, Issue 43, pages 10030-10244, 2022) *2022*

ATPESC 2022 participant under competitive selection *2022*

MRS 2022 NM05 Symposium Best Student Poster Presentation Award winner *2022*

Recipient of TLARGI fellowship *2019*

Teaching/Research Assistant from University of Southern California *2019 - 2022*

Viterbi School of Engineering/Graduate School Fellowship, University of Southern California *2018 - 2019*

Excellent Graduate Award of Beijing *2018*

Excellent Graduate Award of University of Chinese Academy of Sciences *2018*

Meritorious Winner in Mathematical Contest in Modeling *2017*

Merit Student, University of Chinese Academy of Sciences *2017*

Merit Student, University of Chinese Academy of Sciences *2016*

Merit Student, University of Chinese Academy of Sciences *2015*

Excellent Scientific Research Practice Individuals, Chinese Academy of Sciences *2015*

PUBLICATIONS

Published Work

- [1] **Yang, L.**; Jaramillo, R.; Kalia, R. K.; Nakano, A.; Vashishta, P., Pressure-Controlled Layer-by-Layer to Continuous Oxidation of ZrS2(001) Surface. ACS Nano 2023, 17, 8, 7576–7583.
- [2] **Yang, L.**; Nomura, K.; Krishnamoorthy, A.; Linker, T.; Kalia, R. K.; Nakano, A.; Vashishta, P., Surface Transfer Doping in MoO3–x/Hydrogenated Diamond Heterostructure. Journal of Physical Chemistry Letters 2024, 1579-1583.

- [3] Ibayashi, H.; Razakh T. M.; **Yang, L.**; Linker, T.; Olguin, M.; Hattori, S.; Luo, Y.; Kalia R. K.; Nakano, A.; Nomura, K.; Vashishta, P., Allegro-Legato: Scalable, Fast, and Robust Neural-Network Quantum Molecular Dynamics via Sharpness-Aware Minimization. ISC High Performance 2023: High Performance Computing, 223–239.
- [4] **Yang, L.**; Tiwari, S. C.; Fukushima, S.; Shimojo, F.; Kalia R. K.; Nakano, A.; Vashishta, P.; Branicio. P. S., Photoexcitation-Induced Nonthermal Ultrafast Loss of Long-Range Order in GeTe. Journal of Physical Chemistry Letters 2022, 13, 43, 10230–10236.
- [5] Nazarova. A. L.; **Yang, L.**; Kuang, L.; Mishra A.; Kalia R. K.; Nomura K.; Nakano, A.; Vashishta, P., Dielectric Polymer Property Prediction Using Recurrent Neural Networks with Optimizations. Journal of Chemical Information and Modeling 2021, 61, 5, 2175-2186.
- [6] **Yang, L.**; Tiwari, S. C.; Jo, S. S.; Hong, S.; Mishra, A.; Krishnamoorthy, A.; Kalia, R. K.; Nakano, A.; Jaramillo, R.; Vashishta, P., Unveiling Oxidation Mechanism of Bulk ZrS2. MRS Advances 2021, 6, 303-306.
- [7] Chang, Q.; **Yang, L.**; Ge, W., Fluid-Particle Heat Transfer in Static Assemblies: Effect of Particle Shape. International Journal of Heat and Mass Transfer 2021, 166, 120730.
- [8] Jo, S. S.; Singh, A.; **Yang, L.**; Tiwari, S. C.; Hong, S.; Krishnamoorthy, A.; Sales, M. G.; Oliver, S. M.; Fox, J.; Cavalero, R. L.; Snyder, D. W.; Vora, P. M.; McDonnell, S. J.; Vashishta, P.; Kalia, R. K.; Nakano, A.; Jaramillo, R., Growth Kinetics and Atomistic Mechanisms of Native Oxidation of ZrSxSe2–x and MoS2 Crystals. Nano Letters 2020, 20 (12), 8592-8599.
- [9] Xing, W.; Chen, Y.; Wu, X.; Xu, X.; Ye, P.; Zhu, T.; Guo, Q.; **Yang, L.**; Li, W.; Huang, H., PEDOT: PSS-Assisted Exfoliation and Functionalization of 2D Nanosheets for High-Performance Organic Solar Cells. Advanced Functional Materials 2017, 27 (32), 1701622.

In Submission

- [10] **Yang, L.** et al, Quantum Molecular Dynamics Simulations of Protonic Synapse Switching in Hydrogen Doped WO3. (in progress)

In Preparation

- [11] **Yang, L.** et al, Critical ZrS2 Oxidation Moments. (in progress)
- [12] **Yang, L.** et al, Effect of Strain and Metal Doping on Thermal Conductivity of TMDCs. (in progress)

RESEARCH HIGHLIGHTS

- To study the oxidation of ZrS2, a first-principles based ReaxFF force field, was first developed and optimized using multi-objective genetic algorithm. Using the optimized ReaxFF force field, I performed reactive molecular dynamics (RMD) simulations to study the oxidation mechanism of ZrS2. RMD simulations supported by first-principles calculations elucidate the atomistic oxidation mechanisms. This work suggests that oxygen partial pressure is indeed a promising control parameter for such active oxidation for future 2D electronics. We found that ZrS2 has a much higher oxidation rate than MoS2, and that ZrS2 (210) surfaces have a higher oxidation rate than on (001) surfaces. Furthermore, the oxidation process is found to be diffusion-controlled. First-principles calculations show that the initial adsorption of oxygen atoms on the surface is driven by the large binding energy. We find that pressure can selectively expose three stages of oxide growth in the Deal-Grove model within a given time window: (1) Initial incubation, (2) reaction-limited linear growth, and (3) diffusion-limited parabolic growth, with increased pressure. We also find a trade-off between the growth speed and the quality of the grown oxide structure, as well as pressure control of the morphology of semiconductor/oxide interfaces. After an initial stage of slow, layer-by-layer oxidation,

local breakdown of vdW gaps accelerates the diffusion of oxygen, creating a kink-mediated amorphous oxide growth front, with kinetics well described by the conventional Deal-Grove model. The transition time from layer-by-layer to continuous oxidation, as well as that between reaction-limited linear and diffusion-limited parabolic oxidation within the Deal-Grove regime, is well controlled by pressure. Such atomistic elaboration in the well-established Deal-Grove framework is expected to apply to broad TMDC materials, thus rationally guiding experimental growth of vdW heterostructure devices. The ab initio molecular dynamics (AIMD) simulations reveal detailed picture for the oxygen substituting sulfur atoms and oxygen atoms transporting in the bulk.

Published Work:

1. **Yang, L.**; Jaramillo, R.; Kalia, R. K.; Nakano, A.; Vashishta, P., Pressure-Controlled Layer-by-Layer to Continuous Oxidation of ZrS2(001) Surface. ACS Nano 2023, 17, 8, 7576–7583.

2. **Yang, L.**; Tiwari, S. C.; Jo, S. S.; Hong, S.; Mishra, A.; Krishnamoorthy, A.; Kalia, R. K.; Nakano, A.; Jaramillo, R.; Vashishta, P., Unveiling Oxidation Mechanism of Bulk ZrS2. MRS Advances 2021, 6, 303-306.

3. Jo, S. S.; Singh, A.; **Yang, L.**; Tiwari, S. C.; Hong, S.; Krishnamoorthy, A.; Sales, M. G.; Oliver, S. M.; Fox, J.; Cavalero, R. L.; Snyder, D. W.; Vora, P. M.; McDonnell, S. J.; Vashishta, P.; Kalia, R. K.; Nakano, A.; Jaramillo, R., Growth Kinetics and Atomistic Mechanisms of Native Oxidation of ZrSxSe2–x and MoS2 Crystals. Nano Letters 2020, 20 (12), 8592-8599.

- To study the photoexcitation-induced GeTe amorphization, I performed nonadiabatic quantum molecular dynamics (NAQMD) simulations and density functional theory (DFT) calculations. The NAQMD simulations show that nonthermal structural disorder in GeTe occurs after photoexcitation at an excitation level of no less than 4.0%. Accompanying the photoexcitation, we observe the swift charge transfer from Te to Ge atoms. The Mulliken bond overlap show increased Ge-Ge and Te-Te bonding interaction together with weakened Ge-Te bonding interaction. The examination of local disorder at 4.0% excitation level shows the trigger to be a Ge atom diffusion from octahedral to tetrahedral sites. Meanwhile, the excited orbitals are found to be spatially concentrated in the locally disordered region. The electronic density of states calculations show crossings of the Te p to the conduction band and the Ge p to the valence band, together with the crossing of Ge s from the conduction band to the valence band after photoexcitation. The behavior of these crossings combined with band structure analysis suggest that photoexcitation plays an important role on the behavior of the Te p, Ge p, and Ge s electrons. This work sheds light on structural and electronic mechanisms for photoexcitation induced GeTe amorphization and explores the bonding nature during this process.

  Published Work:

  Yang, L.; Tiwari, S. C.; Fukushima, S.; Shimojo, F.; Kalia R. K.; Nakano, A.; Nakano, A.; Vashishta, P.; Branicio. P. S., Photoexcitation-Induced Nonthermal Ultrafast Loss of Long-Range Order in GeTe. J. Phys. Chem. Lett. 2022, 13, 43, 10230–10236.

  (**Cover Image of JPCL (Vol 13, Issue 43, pages 10030-10244, 2022))**

- To investigate the surface transfer doping of Diamond/MoO3-x, I performed RMD simulations and DFT calculations to study the deposition of MoO3-x on hydrogenated diamond (111) surface. A three-step workflow was proposed in this study: (1) Performing RMD simulations to generate the thermalized interfacial structure, (2) employing DFT to further optimize the interfacial structure, (3) conducting DFT calculations to study the electronic structures. The atomistic arrangement is more compact and Mo-O bond is stronger as vacancy level increases. Difference in the Bader charges after deposition reveals the net charge transfer due to deposition. Results show the molybdenum oxides as effective electron accepting materials, which are consistent with experiments. An increase in charge transfer for higher Mo oxidation state is observed, which results in resistance decrease

and current increase in electrical device. This monotonic enhancement in charge transfer as a function of oxidation state provides guidance for engineering the STD process to maximize the charge transfer.

Published Work:

Yang, L.; Nomura, K.; Krishnamoorthy, A.; Linker, T.; Kalia, R. K.; Nakano, A.; Vashishta, P., Surface Transfer Doping in MoO3–x/Hydrogenated Diamond Heterostructure. J. Phys. Chem. Lett. 2024, 1579-1583. DOI: 10.1021/acs.jpclett.3c03541.

(Presentation based on this was selected as **MRS 2022 NM05 Symposium Best Student Poster Presentation Award winner**)

RESEARCH EXPERIENCE

Quantum Molecular Dynamics Simulations of Protonic Synapse Switching in Proton Doped WO3 *2022-2023*

- Performed quantum molecular dynamics simulations and calculations based on density functional theory to study the hydrogen doping in WO3.
- Examined the structure of the doped system and calculated the electrical conductivity, carrier mobility for the doped systems.

Atomistic and Electronic Structures of MoO3-x on Hydrogenated Diamond

- Used RMD to generate thermalized interfacial structures.
- Performed DFT calculations to further optimize this thermalized interfacial structure, and studied the electronic structure and charge transfer at the interface.

Optimization of RXMD-NN Simulator *2022-2023*

- Used Intel-Vtune and Advisor to determine the most compute-intensive function to be optimized.
- Used OpenMP programming to accelerate the RXMD-NN simulator, and performed the weak scaling and strong scaling, and used OpenMP with target offload directive for implementing the GPU version on USC-CARC, and further optimized the GPU version by loop reordering.

Ultrafast Photoexcitation Driven Nonthermal Amorphization of GeTe *2020-2022*

- Performed nonadiabatic quantum molecular dynamics (NAQMD) simulations to study the non-thermal amorphization process in GeTe induced by photoexcitation at various excitation level.
- Found the local disorder mechanism at atomistic and electronic level.

Unveiling Oxidation Mechanism of ZrS2 *2019-2023*

- Developed a first-principles based ReaxFF forcefield, and further optimized the forcefield by using multi-objective genetic algorithm in EZFF forcefield training software.
- Performed RMD and QMD simulations using the developed ReaxFF forcefield to study the oxidation mechanisms of ZrS2 and MoS2.

Heat Transfer in Buckled Transition Metal Dichalcogenide (TMDC) *2019*

- Used non-equilibrium molecular dynamics (NEMD) simulation to simulate the heat transfer in buckled 2D materials.
- Invesitgated in-plane heat transfer in monolayer MoSe2 and WSe2 with strain applied. Examined the combined effect of strain and nanostructure on in-plane thermal conductivity on the alloy W0.11Mo0.89Se2 and heterostructure WSe2/MoSe2.

TEACHING EXPERIENCE

NSF supported CyberMAGICS workshop (Lecturer) *2023 Summer*

PHYS135B: Physics for the Life Sciences (Undergrad course, teaching assistant) *2023 Spring*

PHYS135B: Physics for the Life Sciences (Undergrad course, teaching assistant) *2022 Fall*

NSF supported CyberMAGICS workshop (Helped organize) *2022 Summer*

PHYS135B: Physics for the Life Sciences (Undergrad course, teaching assistant) *2022 Spring*

PHYS135B: Physics for the Life Sciences (Undergrad course, teaching assistant) *2021 Spring*

PHYS135B: Physics for the Life Sciences (Undergrad course, teaching assistant) *2020 Fall*

MASC575: Basics of Atomistic Simulation of Materials (Graduate course, teaching assistant) *2020 Spring*

Being invited to teach middle school students for 1 month *2014 Summer*

CONFERENCE AND WORKSHOP PRESENTATIONS

Oral Presentation:

- Give presentation at CyberMAGICS 2023 *2023 Summer*
- Surface doping of MoO3-x on hydrogenated diamond *2023 APS March Meeting*
- Ab initio molecular dynamics simulation study of oxidation of ZrS2 (001) *2022 MRS Fall Meeting Exhibit*
- Ab initio molecular dynamics simulation study to reveal oxidation mechanism of ZrS2 *CCP 2022*
- Pressure-dependent layer-by-layer oxidation of ZrS2 (001) surface *2022 APS March Meeting*
- Ultrafast photoexcitation driven non-thermal amorphization of GeTe *2021 APS March Meeting*
- Unveiling oxidation mechanism of bulk ZrS2 *2021 MFD Symposium*
- Unveiling oxidation mechanism of bulk ZrS2 and MoS2 *2020 MRS Fall Meeting Exhibit*

Poster Presentation:

- Quantum and reactive molecular dynamic simulations for future semiconductors *2023 MFD Symposium*
- Atomistic and electronic structures of MoO3-x on hydrogenated diamond *2022 MRS Spring Meeting Exhibit*

  (MRS 2022 NM05 Symposium Best Student Poster Presentation Award winner)

SERVICE

Workshop Organization:

- Organize IC2024 meeting *2024*
- Give tutorial on NSF supported CyberMAGICS workshop *2023 Summer*
- Organize NSF supported CyberMAGICS workshop *2022*

Journal Review:

- Review for journal: Computer Physics Communications.

SKILLS

Computing Skills: Machine learning, High Performance Computing (I have been using USC's Center for Advanced Research Computing (CARC) and the Theta machine at the Argonne Leadership Computing Facility (ALCF) to perform Neural Network Molecular Dynamics (NNMD) simulations to examine the computational statistical scalability.)

Programming Skills: MATLAB, Python, C, Fortran, bash

Experienced Softwares: LAMMPS, VASP, RXMD, QXMD, Quantum espresso