Junwei He

Materials Science
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Google Scholar

Education

- **Department of Materials Science and Engineering, UCLA** *Sep 2024 - Jul 2029 expected*
  PhD student in theoretical materials science
- **College of Chemistry and Molecular Engineering, Peking University** *Sep 2020 - Jul 2024*
  Bachelor of Science in Chemistry **GPA: 3.77/4.00**

Research Experience

- **Calculation on the Mechanical and Electrical Properties of t-BN Monolayer** *March 2022 - August 2022*
  Prof. Zhirong Liu's group, Peking University
  - Optimized the lattice constants and crystal structure of tetragonal BN (t-BN), computed the band structure, validated the Dirac Cones via group theory, and determined the anisotropic Fermi velocity analytically.
  - Computed the elasticity coefficients under stress, derived anisotropic Young's Modulus and Possion's Ratio.
  - Calculated the intrinsic carrier mobility using revised deformation potential theory.
- **Tight-Binding Analysis of Dirac Cone Properties in Square–Octagon Lattice** *August 2022 - June 2023*
  Prof. Zhirong Liu's group, Peking University
  - Deduced the Tight-Binding (TB) Hamiltonian for the bipartite square-octagon lattice, obtained an analytical formula to determine the position of the Dirac cone, and analyzed its various properties (anisotropy, tilting, merging, and emerging) based on TB parameters.
  - Applied the "divide-and-couple" method to further understand the origin of Dirac cones.
  - Explored four practical systems using Density Functional calculations and compared results with TB analysis.
- **Molecular Mechanism Calculation of Atomic Substitution of 2D MoS_2 to MoN** *July 2023 - Jan 2024*
  Prof. Boris I. Yakobson's group, Rice University (Collaborated with Prof. Xi Ling, Boston University)
  - Calculated geometrical and electronic structures of reactants and products using VASP, obtained the macroscopic energy changes of the reaction, and explained the need for excess ammonia gas under experimental conditions.
  - Established a simple model for 1D reaction boundaries, identified a unique low-coordination structure at the boundary, and calculated the interfacial energy and micro-scale growth energies.
  - Constructed and optimized a practical 2D propagation model for MoS_2 to MoN conversion, derived a rational 11-step reaction pathway, and calculated energy barriers using CI-NEB method with VTST.

Publications

- **Dirac cones in bipartite square–octagon lattice: A theoretical approach** *July 2023*
  Junwei He and Zhirong Liu, *The Journal of Chemical Physics*, **159**, 044713 (2023)

Technical Skills and Interests

English Proficiency: TOEFL 114 (R30, L30, S25, W29), GRE 336+3.5 (V166, Q170, AW3.5)
Research Skills: General - Python, Linux, Origin, Chemdraw
Professional Software - VASP with VTST/phonony package, Material Studio, Wannier90, Gaussian, VESTA, TB studio, DFTB+.
Proficient in basic VASP calculations, including geometry optimization, band structure, density of states, vibrational frequency, elasticity coefficient, AIMD simulation
Areas of Interest: computational material design, topological materials, machine learning

Awards and Honors

- **Academic Excellence Reward** Peking University *Oct 2022*
- **National Scholarship** Ministry of Education of China *Sep 2023*