Yubi Chen

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Education

University of California, Santa Barbara (UCSB) **September 2019–Now**
Ph.D. of Physics, (GPA:4.00/4.00) *Santa Barbara, US*

- Advisor: Chris G. Van de Walle (2020-2022)
- Current research topic: Defects in wide-gap semiconductors for quantum applications. Formation and control of point defects for experimental realizations.
- Core courses: MATRL 279 First-principles calculations for materials. MATRL 288A Topics in quantum materials. PHYS 217 A/B Many-body problem in condensed matter physics.

University of Chicago **September 2018–June 2019**
Master of Science, (GPA:4.00/4.00) *Chicago, US*

- Advisor: Peter Littlewood
- Research topic: Self-developed code to study electron transport in quantum dot hall effect.
- Core courses: Topological quantum matter. Machine learning. Unsupervised learning and data analysis.

University of Oxford **October 2017–March 2018**
Visiting Student of Physics, *Oxford, UK*

- Core courses: condensed matter physics, quantum atomic and molecular physics, symmetry and relativity, flows and complexity, subatomic physics, and general relativity and cosmology.

University of Chinese Academy of Sciences (UCAS) **September 2014–June 2018**
Bachelor of Physics (GPA:3.91/4.00, Subject GPA:4.00/4.00) , *Beijing, China*

- Advisor: Xiaojun Bi
- Core courses: computational physics, solid state physics, non-equilibrium statistical physics, group theory, quantum field theory, quantum mechanics.

Awards and Scholarship

Quantum Foundry traineeship, 2022-2024 (3 years)
UChicago admission scholarship, 2019 (1/3 tuition).
Merit Student of Beijing.
Scholarship and Merit Student of UCAS, 2014-2018 (4 years).
Model student and excellent student cadre of UCAS.

Research Experience

First-principles study of quantum defects in semiconductors:
(Oct. 2020–Now) *Professor Chris G. Van de Walle*

- Explore the point defects and impurities in BeO as quantum defect candidates. Also, identify how point defects may impact its performance in various applications like protective coating.
- Employ density functional theory (DFT) calculations with a hybrid functional to obtain defect properties like atomic geometries, orbital structures, electronic structures, and optical properties, etc.
- Find that Be and O vacancies are the most stable among native defects in BeO.
- Identify and investigate BeO defects with electron states well separated from the band edges for potential quantum applications like spin qubits or single photon emitters.
- Study whether forming donor-acceptor complex can promote the properties of quantum defect candidates, such as expanding the Fermi level stability range and reducing the electron-phonon coupling.

Hydrogen migration in diamond:
(Apr. 2022–Now) *Professor Chris G. Van de Walle*

- Identify that hydrogen migration in diamond has inconsistent results in literature.
- Calculate hydrogen impurity ground states in different charges with a DFT hybrid functional.
- Explore the hydrogen migration paths by climbing image nudged elastic band method, and find the migration path with lowest migration barrier.
- Obtain hydrogen migration barriers for different charge states. Find that H in positive charge state has a tiny migration barrier compared to its neutral and negative charge states, indicating that avoiding positively-charged hydrogen could potentially reduce the concentration of desired quantum defects like diamond NV center.

Effective magnetic-phonon interaction:
(Nov. 2019–Aug, 2020) *Professor Leon Balents*

- Derived magnetic-elastic interaction from magnetic dipole interaction with distortions.
- Derived the effective magnetic-phonon interaction by integrating out magnetization from a Berry phase term (magnetization-magnetic-field interaction) and magnetization-elastic interaction.
- Derived the Hamiltonian of acoustic phonons of an isotropic medium under a magnetic field from first principles, which is not present in current literature.

Electron Transport: **University of Chicago**
Master's Project (Nov. 2018–May, 2019) *Professor Peter Littlewood*

- Obtained the Hall effect for mercury chalcogenide colloidal quantum dot films using ensemble average of electron variable-range-hopping simulation on a 2-d lattice with disorder under a magnetic field.
- Used continuous-time-random-walk algorithm to expedite the simulation with a low hopping probability, which is a great improvement compared to Monte Carlo method.

Genome Segmentation and Viral RNA packing: **Institute of Physics**
Summer Research (May 2018-Aug. 2018) *Professor Rudolf Podgornik*

- Simulated a coarse-grained model of icosahedral viruses using molecular dynamics simulations, yielding certain packing motifs of RNA-polymer Lambert-projection distribution.
- Developed a method to explain RNA distribution motifs and verified this method by its predictions.
- Extended physical picture of this method to explain new motifs with different characteristics successfully.
- Quantified those motifs through spherical-harmonic-function projection, with peak positions and peak heights exactly agreeing with the predictions.

Construction of Electron Energy Spectrum: **Institute of High Energy Physics**
Bachelor's thesis (Mar. 2018-Jun. 2018) *Professor Xiaojun Bi*

- Compared the effects of different machine learning classification methods, such as direct cut and boost decision tree (BDT) algorithms. Obtained a 99.97% electron-background-removal rate using BDT.
- Analyzed the influences of partition methods and obtained a good energy-bin partition that can both maintain low errors and obvious spectrum fine structures.
- Analyzed spectrum peak stability against energy-bin partition being used by Particle Astrophysics Division to get energy spectrum with high accuracy.

Emissivity Measurements: **University of Oxford**
Group project (Nov. 2017-Mar. 2018) *Professor John Malcolm*

- Fabricated and characterized samples with different surfaces and verified the relation between roughness, reflectivity and emissivity resembled Agababov model.
- Proposed fitting the spectrophotometer with an integrating sphere to reduce diffuse light, and measured emissivity more accurately in shock experiments.
- Found the dramatically-negative effect of Lithium Fluoride windows used in shock experiments on emissivity measurements.

High Energy Theory: **Institute of High Energy Physics**
Research experiences (Jun. 2017-Aug. 2017) *Professor Yu Jia and Xiaojun Bi*

- Solved the Klein-Gordon equation with low-dimensional Hydrogen potential and used anti-particle concept from Quantum Field Theory to explain Klein paradox.
- Simulated Dark Matter freeze-out from the Boltzmann Equation based on Four-Fermion interaction between Dark Matter and Standard Model fermions, yielding Dark Matter relic density.

Fundamentals of Experimental Microgravity: **Institute of Mechanics at CAS**
Research Project (Jun. 2016-Jul. 2016) *Professor Qi Kang*

- Reconstructed Micro-Propulsion measurement devices, which can measure weak force from milli-Newton to micro-Newton, designed for Chinese Gravitational-wave Detection Satellites.
- Measured Torsion Balance Micro-Propulsion measurement devise with a Laser Displacement Sensor. Analyzed tripod vibration data and obtained vibration spectrum.

The critical phenomena of Casimir Effect: **Institute of Theoretical Physics**
Course Project (Apr. 2016-Jun. 2016) *Professor Xiaosong Chen*

- Proposed a new method to calculate the grand potential in Momentum Space, and obtained free energy by Poisson summation and Cauchy Integration.
- Found that the singularity in partition function at the zero-momentum point is lost in integration.
- Added a finite size correction term depending on the scale of Casimir system near the critical limit.

Publication

Chen Y., Turiansky M. E., and Van de Walle C. G., First-principles study of quantum defect candidates in beryllium oxide, submitted to PRB.
Chen Y., Wang M., and Van de Wale C. G., Hydrogen migration in diamond, in preparation

Presentations

Contributed talks

- Beryllium oxide as a host for quantum defects. Thrust 3 meeting, quantum foundry. Santa Barbara. April 8th, 2022.
- Beryllium oxide as a host for quantum defects. March meeting, American Physical Society. Chicago. March 17th, 2022.
- First-principles calculations of native defects in beryllium oxide. March meeting, American physical society. Online. March 18th, 2021.
- First-principles calculations of native quantum defects in beryllium oxide. Graduate Simulation Seminar Series, UCSB. Online. July 14, 2021.

Poster presentation

- First-principles studies of quantum defects. Quantum industry showcase, Quantum Foundry. UCSB. April 22nd, 2022.
- First-principles studies of quantum defects. All hands meeting, Co-design Center for Quantum Advantage (C2QA). UCSB. Feburary 25th, 2022
- First-principles modeling of defects in materials for quantum information science. All Hands Meeting, Brookhaven National Lab. Online. November 10th, 2021

Teaching experience

Teaching assistant at UCSB (undergraduate level courses in department of physics)

- Phys 104 Advanced mechanics *2022 Winter*
  Lagrangian mechanics. Hamiltonian mechanics, etc.
- Phys 103 Intermediate mechanics and special relativity *2021 Fall*
  Newtonian mechanics in 3D. Conservation laws. Oscillations. Scattering. Special relativity.

- Phys 25 General physics *2021 Spring*
  Blackbody radiation. Compton scattering. Bohr model. Quantum mechanics. Nuclear physics.
- Phys 119B Thermal and statistical physics *2021 Winter*
  Statistical mechanics: Boltzmann, Fermi-Dirac, and Bose-Einstein distribution.
- Phys 110A Electromagnetism *2020 Fall*
  Electrostatics. Laplace's equation. Magnetostatics. Electric and magnetic fields in matter.
- Phys 22 General physics *2020 Spring*
  Temperature and heat, the laws of thermodynamics, wave interference and normal modes.
- Phys 20 General physics *2019 Fall*
  Classical mechanics. Kinematics. Vectors. Newton's laws. Work and energy. Conservation laws.

Programming Skills

Proficient: VASP, Python, Linux, Shell, Mathematica, TeX, Vesta.
Intermediate: C, Fortran, Root, Lammps, Matlab.
Novice: Visual Molecular Dynamics, Quantum Espresso.