We develop theoretical and computational methods to predict and engineer material and molecular properties from first principles.

Spin Quibits for Quantum Information Technologies

We aim to understand the atomic and electronic structure of spin defects in semiconductors and their coherence properties.

We predict novel defects as platforms for quantum information processing.

As a part of: QISpin project, Chicago MRSEC Q-NEXT hub, Chicago Quantum Exchange and NSF center QuBBE.

Materials for: Sustainable Energy Sources Quantum Technologies

Methods and Code Development

We develop methods based on quantum mechanics and open-source software to understand and predict the properties of solids and molecules at the microscopic scale.

Methods:

First Principles Molecular Dynamics

Many Body Perturbation Theory

Quantum Embedding Theory

Cluster-Correlation Expansion

PyCCE

We partake in the Midwest Integrated Center for Computational Materials (MICCoM) to couple codes at different scales and develop strategies for data curation and availability.

Enforce particle number conservation through post selection over measurements to obtain physical results.

We use Quantum Embedding Theory to simulate the eigenstates of spin defect systems with variational quantum Eigensolver (VQE) on IBM quantum computers.

Coherence Properties of Spin Quibits

We uncover substrate effect on coherence in 2D materials.

We study spin dynamics of divacancies in SiC at avoided crossings.

We combine DFT electronic structure and CCE calculations to characterize coherence time of nuclear spins in the frozen core of NV center in diamond.

Computational Scoposcopy of Spin Defects

We develop ab initio approaches to compute vibrationally resolved optical spectra of point defects in semiconductors.

We implement excited state analytical forces for TDDFT, spin-flip, in the WEST code.

We investigate the vibrationally resolved photoluminescence, excitation, and photo-ionization spectra of spin-defects in semiconductors.

Research Overview

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