Physics-Informed Machine Learning and Quantum Mechanics for Electronic Structures and Molecular Spectroscopy

Seminar

Monday

Sept. 14, 2026

3:00 – 4:00pm

Beaupre Center, Room 105

Prof. Zhou Lin

Univ. of Massachusetts, Amherst

Our research encompasses forward structure-to-property prediction and inverse property-to-structure inference and provides essential tools for predicting and interpreting molecular structures and dynamics. We are developing computational models that combine physics-informed machine learning with quantum mechanics for these goals.

To achieve high-throughput inference of spectroscopic signals without trial and error, we created Spec2D, an encoder–decoder architecture that translates spectroscopic signals into molecular identity and connectivity. This process uses pre-trained large language models, such as transformers and GPT, to treat the task as a form of language translation. Spec2D demonstrates state-of-the-art accuracy in inferring the structures of single molecules and binary mixtures from calculated and experimental IR, NMR, and mass spec signatures.

To predict electronic structures and UV–vis spectra of organic semiconducting molecules and radicals, we developed ML-ωPBE, a machine-learned, range-separated density functional. This functional determines the range separation parameter, ω, directly from semi-empirical geometric and electronic features through regression and graph neural network models. ML-ωPBE outperforms all widely used functionals in predicting spectroscopic properties and requires no modifications when adopted to molecular aggregates and radicals.

To analyze fragment–fragment and fragment–environment interactions of complex systems, we developed FB-GNN-MBE, a hybrid quantum mechanics/machine learning method. This approach evaluates energies, forces, and energy components of a system using many-body expansion theory and fragment-based graph neural networks. FB-GNN-MBE accurately reproduces first-principles full-dimensional and reduced-dimensional potential energy surfaces of non-covalently bonded molecular clusters within chemical accuracy.

In summary, our research has advanced the field of electronic structures and molecular spectroscopy by improving the fidelity of electronic structures for molecules and radicals, automating structural inference from spectroscopic signals, and enabling scalable modeling of condensed phase environmental effects.

THE UNIVERSITY OF RHODE ISLAND

Department of Chemistry

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