Inference based model Hamiltonians balancing accuracy, interpretability and data efficiency.

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Predicting electronic structure efficiently and accurately remains a major challenge for large and complex systems. While deep learning has made significant strides in this area, it often requires vast datasets and sacrifices interpretability. This talk presents an inference-based approach that balances accuracy, interpretability, and data efficiency - an approach we refer to as "shallow learning."

Our method constructs model Hamiltonians by representing the electronic manifold using quasi-atomic orbitals and expanding operators with multi-center integrals. This framework enables a smooth transition from plain two-center tight-binding models to full ab initio representations, offering both efficiency and flexibility. Additionally, we incorporate soft orthogonality and localization constraints, ensuring physically meaningful results while maintaining computational efficiency.