Equivariant AI-based models for accurate electronic Hamiltonians

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Modern density functional theory (DFT) has reached a high level of predictive power. When coupled with advanced simulation techniques—such as linear-scaling quantum transport methods—it becomes, in principle, possible to predict a material's electronic properties directly from its atomic structure. This capability is laying the foundation for what is increasingly referred to as *materials digital twins*. However, *ab initio* methodologies remain computationally demanding and are typically limited to relatively small, pristine systems with minimal disorder. This is a significant limitation, as disorder plays a critical role in electronic transport and often governs the functional limits of a material's electrical performance.

While transport methodologies can scale to systems with billions of orbitals, the primary bottleneck lies in generating the Hamiltonian used as input. In this context, machine learning (ML) has emerged as a promising tool to bypass traditional *ab initio* calculations. In this talk, we will focus on *equivariant models*—a class of ML architectures that preserve the fundamental symmetry transformations of physical systems. These models are especially relevant in areas such as orbitronics and spintronics, where symmetry considerations govern allowed orbital configurations and spin–orbit coupling plays a central role in the physical behavior. We will discuss recent progress and open challenges in using equivariant neural networks to construct accurate, symmetry-aware Hamiltonians for large-scale quantum transport simulations.

References

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