First-Principles Many-Body Theory and Quantum Dynamics for Materials in Quantum Information Science

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Stable, scalable, and reliable quantum information science (QIS) is poised to revolutionize human well-being through quantum computation, communication and sensing. In this talk, I will show our recent development on first-principles computational platforms to study quantum coherence and optical readout as critical processes in QIS and spintronics in solid-state materials, by combining first-principles many-body theory and open quantum dynamics.

First, we will show how we reliably predict energetics, electronic and optical properties of spin defects and their host two-dimensional materials from first-principles many-body theory, which accurately describes highly anisotropic dielectric screening and strong many-body interactions. In particular, we will show how we predict spin-dependent optical contrast for information readout of spin qubits by computing exciton radiative and phonon-assisted nonradiative as well as spin-orbit induced intersystem crossing rates from first-principles.

Next, we will introduce our recently developed real-time density-matrix dynamics approach with first-principles electron-electron, electron-phonon, electron-impurity scatterings and self-consistent spin-orbit coupling, which can accurately predict spin and carrier lifetime and pump-probe Kerr-rotation signatures for general solids. As an example, we will show our theoretical prediction on Dirac materials under electric field with extremely long spin lifetime and spin diffusion length, and distinct dependence on electron-phonon couplings in spin and carrier relaxation in halide perovskites. This theoretical and computational development is critical for designing new materials promising in quantum-information science and spintronics applications.