

Real-time time-dependent density functional theory calculations of spin-orbit dynamics and Berry-curvature characteristics of solid states

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We have used the real-time time-dependent Kohn-Sham equations, within adiabatic local density approximation, to reveal various Berry-curvature characteristics of solid states. We successfully demonstrated that the quantum anomalous Hall conductivity and the quantum spin Hall conductivity of real-material bulk topological insulators can be directly obtained in the real-time profile. We now extend our study to nonlinear optical responses associated with spin-orbit dynamics. We particularly focus on the structures with the built-in geometrical chirality. When such a chiral structure is exposed to an axial magnetic field, the consequent charge dynamics exhibits sharply analogous responses as the axial anomaly of high-energy physics of massless fermions. We discuss the limitation and utility of local spin density approximation for the exchange-correlation magnetic field in the aforementioned spin-orbit dynamics.