Density-functional-theory calculations of currents in real materials and the study of topological & geometrical nature of band states or other physical systems

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We have explored charge and spin currents in real materials using ***ab initio*** computational methods, grounded in Time-Dependent Density Functional Theory (TDDFT) and Time-Dependent Current Density Functional Theory (TDCDFT). While our research has examined various Berry curvature characteristics in solid-state systems, our primary focus is on uncovering the topological and geometrical properties of band states in the real-time dynamics of materials. For instance, we show that quantum anomalous Hall conductivity and quantum spin Hall conductivity in bulk topological insulators can be directly computed via ***ab initio*** evaluations of charge and spin currents, respectively. In this talk, we also present our recent advances in the study of one-dimensional topological structures, with a particular focus on how the intricate interplay between geometrical helicity, spin-orbit coupling, and conducting charges gives rise to unique spin dynamics, potentially linked to a spin-based counterpart of the Thouless pump.