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Valley Prize Talk

IVO SOUZA, University of California, Berkeley, and Lawrence Berkeley National Laboratory

Intuitively, electrons in metals are "free," while in insulators they are "bound," or "localized." This is why under a dc bias metals carry a steady current and insulators acquire an electric polarization. What is the precise nature of this localization, in view of the fact that the charge density can be as delocalized in a covalent crystal as in a metal? I will discuss a rigorous notion of localization in the insulating state, and how it relates to both the extended ("band") and the localized ("bond") pictures of electrons in solids. It is closely tied to the finding that a knowledge of the bulk charge density alone is not sufficient to define the dielectric polarization. Instead, this quantity is given by a global phase property (Berry's phase) of the Bloch states in the filled bands or, alternatively, by the centers of charge of the occupied Wannier orbitals. Similarly, electron localization in insulators is not a property of the charge density. It is instead related to the spatial extent of the Wannier orbitals, and describes the quantum fluctuations of the ground state polarization. These ideas have had a practical impact on *ab initio* studies of the dielectric properties of real materials. For example, they have led to a method for applying finite electric fields to insulators without resorting to artificial sawtooth potentials.