Wannier Functions for Locally Probing Dielectric and Spectral Properties

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Two developments originating from the concept of maximally localized Wannier functions are discussed. In the first one, maximally localized Wannier functions are used within a theoretical scheme for determining local permittivities [1,2]. The local permittivity is obtained from the microscopic charge density induced by an applied electric field. By analyzing the permittivity in terms of maximally localized Wannier functions, we can relate variations of the microscopic dielectric response to specific features of the local bonding arrangement. The potential of our scheme is illustrated through an application to the permittivity of Si slabs of finite thickness [1]. Our approach indicates that the local permittivity in the slab interior approaches the corresponding value for bulk Si within a few atomic layers from the surface. Therefore, the decrease of the average slab permittivity with thickness originates from the lower permittivity of the outer planes and the increasing surface-to-volume ratio. In the second development, following up with a suggestion of Gygi *et al.* [3], we go beyond maximally localized Wannier functions to construct a partitioning of the electronic structure in terms of functions which simultaneously provide an approximate diagonalization of the Hamiltonian and the position operator [4]. These functions, that we call mixed Wannier-Bloch functions, carry both spatial localization and limited spectral broadening, and are therefore particularly convenient to associate specific spectral features to the underlying atomic-scale mechanisms. By introducing a lattice position operator analogous to the electronic Berry-phase position operator, Wannier-Bloch functions can trivially be extended to the analysis of vibrational modes [4]. Application to vitreous SiO_2 demonstrates that mixed Wannier-Bloch functions constitute a powerful tool for tracking fingerprints of short- and medium-range structural order in electronic and vibrational spectra [4].

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