

## Exploiting orbital localization in electronic structure calculations of complex systems

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Abstract: We discuss algorithms for the computation of electronic properties of complex systems including liquids and solid-liquid interfaces. First-principles simulations and calculations of guasiparticle energies and optical excitation spectra can be performed at various levels of theory, ranging from hybrid density functional theory (hybrid-DFT) to the GW and BSE approximations. The high cost of these calculations motivate approximations based on Kohn's nearsightedness principle that states that most insulating systems can be described in terms of exponentially localized one-particle orbitals within Density Functional Theory. We discuss the use of Maximally Localized Wannier functions and of the method of Recursive Subspace Bisection to obtain localized representations for the computation of electronic properties and molecular dynamics simulations using hybrid density functionals and for the solution of the GW-BSE equations, leading to efficient computation of quasiparticle and optical absorption spectra.

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