Making Mountains out of Molehills, and Other Tails of Disentanglement

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Maximally-localized Wannier functions (MLWFs) can be used as building blocks for the electronic-structure of complex and realistic nanostructures [1,2]. Two broad alternatives are envisioned: 1) MLWFs can act as a minimal basis set, alternative to LCAO, onto which the Hamiltonian is diagonalized with or without a self-consistent update of the charge density, or 2) the Hamiltonian in the MLWFs representation can be directly constructed from the short-ranged Hamiltonians of smaller constituent units, taken either as molecular or periodically-repeated fragments.

In all cases, a robust strategy for constructing MLWFs spanning both the occupied and unoccupied orbitals is required; we'll discuss here examples and applications drawn from the study of pristine and functionalized carbon nanotubes, silicon and silicon-germanium nanowires, and DNA helices [3].

[1] Y.-S. Lee, M. B. Nardelli, and N. Marzari, Phys. Rev. Lett. **95**, 076804 (2005).

[2] Y.-S. Lee and N. Marzari, Phys. Rev. Lett. **97**, 116801 (2006).

[3] A. Mostofi and N. Marzari, in preparation (2007).