

A Localized Orbital Approach to the Correlation Hole and Correlation Energy in Si

Antonio C. Cancio and M. Y. Chou
School of Physics, Georgia Tech, Atlanta GA 30332

With the increasing popularity of exact-exchange and hybrid methods in density functional theory, there is a need to develop improved methods of treating the correlation energy. We study one possible approach to an improved correlation energy calculation in semiconductors by using an expansion of the correlation hole in terms of localized orbitals. We use both maximally localized Wannier functions¹ and orthogonalized LCAO orbitals to describe bonding (valence) and antibonding (conduction) states localized on each bond site. A perturbational configuration-interaction calculation shows that the basic qualitative features of the “left-right” or bond polarization correlation observed in recent variational Monte Carlo calculations of the correlation hole of Si² can be captured with a very small basis of excited states. We discuss preliminary attempts to construct hybrid correlation holes, splining between a detailed orbital description of correlation at longer range and the on-top hole from the local density approximation. The results show promise, but point to the need for a more quantitative calculation of the long-range correlation.

¹N. Marzari and D. Vanderbilt, Phys. Rev. B **56**, 12847 (1997)

²R. Q. Hood et al., Phys. Rev. B **57**, 8972 (1998).