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Maximally-localized Wannier functions for GW quasiparticles
D.R. HAMANN, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University — Recent efforts carrying the GW many-body approximation to self-consistency have given improved electronic-structure results.[1] However, one is left with self-energy operators only on the grid of **k** points used for Brillouin-zone integration, unlike the case of DFT where the local self-consistent potential allows calculation of the band structure on arbitrary **k** points (e.g., along symmetry lines). As maximally-localized Wannier functions[2] (MLWF) provide a basis for a highly accurate approach to band interpolation, we have combined the WANNIER90 code for MLWF with the self-consistent GW capabilities of the ABINIT code to efficiently extend the GW grid calculation to a full band structure. MLWF also provide an intuitive picture of the orbital character and bonding of groups of bands, as well as a quantitatively accurate measure of electric polarization.[2] Differences between quasiparticle[3] MLWF and their LDA counterparts examined to date (Si and perovskite $SrZrS_3$) have proven small, but the visualization of significant many-body effects through MLWF remains an intriguing possibility. 1. F. Bruneval *et al.*, Phys. Rev. B **74**, 045102 (2006). 2. N. Marzari and D. Vanderbilt, Phys. Rev. B **56**, 12 847 (1997). 3. M. van Schilfgaarde *et al.*, Phys. Rev. Lett. **96**, 226402 (2006).

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