Abstract Submitted
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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] Maximally-localized Wannier functions[2] formed from the quasiparticle wave functions[3] provide an efficient and highly accurate basis for interpolating the SCGW bands from a coarse Brillouin-zone mesh to symmetry lines. Since the MLWF's correspond to chemists' bond orbitals, they potentially also provide insight into the qualitative effects of the improved treatment of correlations in SCGW compared to LDA. We report results on $SrTiO_3$, solid Ar, and molecular CO. Band interpolation is accurate and effective for both solids. Small shifts in the degree of hybridization can be visualized for some of the $SrTiO_3$ and CO MLWF's. In Ar, individual conduction-band Bloch functions were found to have large differences between LDA and SCGW.[1] However, a manifold of 9 d and spd-hybrid MLWF's which proved to be the minimum necessary for the lower conduction bands showed minimal differences in the two cases. A fully-functional interface to the WANNIER90 library within the SCGW-capable ABINIT code has been implemented and will be publicly available in the near future. 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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