

Abstract Submitted
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Using Hartree-Fock pseudopotentials in GW calculations D.R. HAMANN, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University — The issue of including shallow “semi-core” states as valence has recently resurfaced in the context of self-consistent GW calculations.¹ Supposing that semi-core-valence exchange is the dominant process necessitating the inclusion of semi-cores, we have investigated whether the use Hartree-Fock pseudopotentials² instead of density-functional psp’s might obviate the need for semi-cores. The answers to this question appear to be “yes” for the case of CuCl (filled d shell), and “semi-cores don’t matter anyway” for ScN (empty d shell). Opportunity permitting, additional examples will be discussed.

¹F. Bruneval *et al.*, Phys. Rev. Lett. **97**, 267601 (2006).

²W. A. Al-Saidi, E. J. Walter, and A. M. Rappe, Phys. Rev. B **77**, 075122 (2008).

D.R. Hamann
Department of Physics and Astronomy, Rutgers University

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