

Abstract Submitted
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Spin-Orbit Effects in the Quasiparticle Bandstructure of Noble Metals¹ JAMAL MUSTAFA, STEVEN LOUIE, Univ of California - Berkeley — Applications of the GW approximation to the electron self-energy have proven quite successful for calculating the quasiparticle properties of materials. We find that for the noble metals, in line with previous work in such calculations, the semicore states need to be taken into account. We show that, with these semicore states, a large cutoff must be used to describe the screening and, in turn, a large number of empty states must be included. Taking all of this into account, and carefully checking convergence, shows G_0W_0 can describe experimental results from angle-resolved photoemission spectroscopy quite well when the effects of spin-orbit coupling is also included. We compare our results to recent self-consistent GW calculations on gold.

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