Abstract Submitted
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First-principles calculations of quasiparticle energies of open-shell condensed matter systems[1] JOHANNES LISCHNER, UC Berkeley and Lab Berkeley National Lab, JACK DESLIPPE, UC Berkeley, MANISH JAIN, STEVEN G. LOUIE, UC Berkeley and Lab Berkeley National Lab — We present a Green's function approach to quasiparticle excitations of open-shell systems within the GW approximation. It is shown that accurate calculations of the characteristic multiplet structure require a precise knowledge of the self energy and, in particular, its poles. We achieve this by constructing the self energy from appropriately chosen mean-field theories on a fine frequency grid. We present results for the nitrogen dioxide molecule and the negatively charged nitrogen-vacancy defect in diamond, which are in good agreement with experiment and other high-level theories.

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