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Plasmon-pole models affect band gaps in GW calculations PAUL LARSON, ZHIGANG WU, Colorado School of Mines — Density functional theory calculations have long been known to underestimate the band gaps in semiconductors. Significant improvements have been made by using GW calculations that uses the self energy, defined as the product of the Green function (G) and screened Coulomb exchange (W). However, many approximations are made in the GW method, specifically the plasmon-pole approximation. This approximation replaces the integration necessary to produce W with a simple approximation to the inverse dielectric function. Four different plasmon-pole approximations have been tested using the tight-binding program ABINIT: Godby-Needs, Hybertsen-Louie, von der Linden-Horsch, and Engel-Farid. For many materials, the differences in the GW band gaps for the different plasmon-pole models are negligible, but for systems with localized electrons, the difference can be larger than 1 eV. The plasmon-pole approximation is generally chosen to best agree with experimental data, but this is misleading in that this ignores all of the other approximations used in the GW method. Improvements in plasmon-pole models in GW can only come about by trying to reproduce the results of the numerical integration rather than trying to reproduce experimental results.

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