Exchange-Correlation in Screened-Exchange Density Functional Methods

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We present a systematic study on the exchange-correlation effects in screened-exchange local density functional method (sX-LDA). To investigate the effects of the screened-exchange potential in the band gap correction, we have compared the exchange-correlation potential term in the sX-LDA formalism with the self-energy term in the GW approximation. It is found that the band gap correction of the sX-LDA method primarily comes from the downshift of valence band states, resulting from the enhancement of bonding structure and the increase of ionization energy. The band gap correction in the GW method, on the contrary, comes in large part from the increase of the conduction band energies. We also studied the effects of the screened-exchange potential in the total energy by investigating the exchange-correlation hole. When the Thomas-Fermi screening is used, the sX-LDA method overestimates (underestimates) the exchange-correlation hole in short (long) range. ¿From the exchange-correlation energy analysis we found that the LDA method yields better absolute total energy than sX-LDA method.