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**Correlation Effects in Screened-Exchange Density Functional Theory** BYOUNGHAK LEE, Lawrence Berkeley National Lab, LIN-WANG WANG, Lawrence Berkeley National Lab — While it has been demonstrated that the screened-exchange local density approximation (sX-LDA) gives good agreement with experiment for fundamental energy gaps of many semiconducting systems, the underlying physics is not always clear. One particular question is, in semiconductor systems, whether the screening should be short range (e.g., the Thomas-Fermi screening) or long range (e.g., by the semiconductor dielectric function). To investigate this, we have compared the self-energy term in the sX-LDA formalism with the self-energy term in the GW approximation and the exchange-correlation hole of variational quantum Monte Carlo simulations. We have also tested the band gaps and total energy results within the sX-LDA formalism with different screening models. The sX-LDA calculations are done using norm-conserving pseudopotentials and a plane-wave basis.

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