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Investigating doping effects in III-nitride materials by large-scale hybrid-functional calculations YING-CHIH CHEN, QING SHI, VINCENT MICHAUD-RIOUX, HONG GUO, McGill University — Electronic properties of semiconductors is strongly influenced by the presence of dopants. Large supercells having over a thousand atoms need to be calculated for dopant concentration below 1% in standard density functional theory (DFT). To deal with the band gap issue of DFT with local/semilocal functionals, the hybrid-functional which mixes the exact exchange (EXX) with semilocal correlation, is often an effective approach. However, performing hybrid-functional simulation with large number of atoms is a challenge. To this end, we have implemented EXX in the framework of numerical atomic orbital (NAO) and pseudopotential which allows us to accurately calculate electronic structures of semiconductors with very small doping concentrations. We show that, (i) the calculated band gap and band structure of semiconductors are accurately comparable with plane-wave and projector augmented wave methods; and (ii) the band gap is nonlinearlly depended on the doping-concentration from 0.1% to 3% in gallium-nitride (GaN) crystals. The numerically very efficient NAO hybrid-functional approach is powerful for investigating semiconductor materials whenever the supercell contains more than several hundred atoms and beyond.

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