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Combining quasiparticle energy calculations with exact-exchange density-functional theory PATRICK RINKE, CHRISTOPH FREYSOLDT, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, ABDALLAH QTEISH, Yarmouk University, Irbid - Jordan, JÖRG NEUGEBAUER, University of Paderborn, Germany — We present a systematic *ab initio* study of the electronic structure for selected II-VI compounds and group III nitrides in the zinc-blende structure with special emphasis on analysing the role played by the semicore *d*-electrons. We show that applying density-functional theory (DFT) in the exact-exchange (EXX) approach [1] leads to an improved description of the *d*-electron hybridisation compared to the local-density approximation (LDA). Moreover we find that it is essential to use the newly developed EXX pseudopotentials [2] in order to treat core-valence exchange consistently. In combination with quasiparticle energy calculations in the *GW* approximation we achieve very good agreement with available photoemission data. Since the DFT energies and wavefunctions serve as input for the *GW* calculation we conclude that for these materials EXX constitutes the better starting groundstate.

[1] M. Städele *et al*, Phys. Rev. Lett. **79** 2089 (1997)

[2] M. Moukara *et al*, J. Phys.: Condens. Matter **12** 6783 (2000)

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