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**The band gap of InN and ScN: a quasiparticle energy study based on exact-exchange density-functional theory** PATRICK RINKE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin - Germany, ABDALLAH QTEISH, Yarmouk University, Irbid - Jordan, JÖRG NEUGEBAUER, MPI für Eisenforschung, Düsseldorf - Germany — The group-IIIA nitride InN and the group-IIIB nitride ScN have recently received increased attention in the field of opto-electronics and optical coatings. Due to the difficulty of growing clean samples, however, the size of their band gap has not been well established, yet. We have recently shown, that quasiparticle energy calculations in the $G_0W_0$ approximation based on density-functional theory (DFT) calculations in the exact-exchange (EXX) approach yield band gaps in very good agreement with experiment for GaN and II-VI compounds [1]. For wurtzite InN our approach predicts a gap of 0.7 eV, suggesting an intrinsic value at the lower end of the experimentally observed range [2]. For ScN there exists a longstanding controversy if the material is a semimetal or semiconductor, which has only very recently been resolved in favor of the latter. Our calculations for rocksalt ScN predict an indirect band gap of 0.9 eV in good agreement with recent experimental findings [3].
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