

Exact-exchange based quasiparticle energy calculations applied to (transition) metal nitrides: ScN, InN and more

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The metal nitride InN and the transition metal nitride ScN have recently received increased attention in the field of opto-electronics. Their electronic band structure – a key quantity for devices – has been difficult to access experimentally (due to growth related problems) and theoretically (due to strong self-interaction effects in the local-density approximation (LDA) to density functional theory (DFT)). Here we show that removing the self-interaction by applying DFT in the exact-exchange optimized effective potential approach (OEPx) correctly predicts ScN and InN to be semiconductors and not (semi)metals as found in the LDA. The OEPx ground state then provides a suitable starting point for quasiparticle energy calculations in the G_0W_0 approximation. Our OEPx+ G_0W_0 gap supports recent experimental observations [1] that ScN has a much lower indirect band gap than previously thought [2]. We further show how a meaningful comparison to LDA based G_0W_0 calculations can be constructed that allows us to make contact with self-consistent GW calculations. For InN our OEPx+ G_0W_0 band gap of 0.7 eV [3] suggests an intrinsic value at the lower end of the experimentally observed range [4]. Taking the Burnstein-Moss effect into account, the increase of the apparent quasiparticle gap with increasing electron concentration is in good agreement with the observed blue shift of the experimental optical absorption edge. Moreover, the concentration dependence of the effective mass, which results from the non-parabolicity of the conduction band, agrees well with recent experimental findings [3,4].

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