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Exact-exchange based quasiparticle energy calculations applied to (transition) metal nitrides: ScN, InN and more P. RINKE, M. SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin - Germany, A. QTEISH, Yarmouk University, Irbid - Jordan, J. NEUGEBAUER, for Iron Research, Düsseldorf - Germany — The transition metal nitride ScN is emerging as a versatile material for promising technological applications, e.g. in spintronics and optoelectronics. Like for InN the electronic band structure of ScN – 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.

[1] A. A. Al-Britthen *et al.*, Phys. Rev. B **70**, 045303 (2004)

[2] P. Rinke *et al.*, cond-mat/0611435

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