Electronic structure of some wurtzite semiconductors: hybrid functionals vs. *ab initio* many-body calculations

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9.7 cm

Using the first-principles projector augmented wave method the structural and electronic properties of wurtzite crystals, AlN, GaN, InN and ZnO have been calculated. The structural parameters have been calculated within different exchange-correlation approximation: DFT, DFT+U and hybrid HSE. The error in the calculated lattice constants are less than 3% within DFT and DFT+U approximations and only 0.5% within HSE. The band gap has been calculated within different GW approximations: G_0W_0, GW_0 - where the eigenvalues in Green's function (G) are updated, GW - where both Green's function and dielectric matrix are updated until self-consistency. The best agreement with experiment was obtained for the GW approximation (see table below). The DFT+U+G_0W_0 gives similar results to GW. The density of states for mentioned compounds have been calculated within DFT, DFT+U and hybrid functional approximation.

Semic.	GGA	GGA+U	HSE06	G_0W_0	U+G_0W_0	GW_0	GW	Exp.
ZnO	0.793	1.403	2.499	2.334	3.152	2.871	3.640	3.430
AlN	4.095	-	5.714	5.523	-	5.780	6.226	6.190
GaN	1.774	2.489	3.348	2.911	3.777	3.110	3.448	3.500
InN	-0.160	0.000	0.772	-	-	-	-	0.7-0.8

13.4 cm

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