Correlation between structural change and electrical transport properties of indium nitride under high pressure

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Supplementary Information for Publication

Table S1. Values of E_g and dE_g/dP for the different candidate phases of InN and the phase transition pressures. B1, B2, and B3 represent the rocksalt, wurtzite, and zinc-blende phase of InN, respectively.

Compound	**Phase**	**Pressure (GPa)**	**E_g (eV)**		**dE_g/dP (meV/GPa)**	
			Present work	**other calculation**	**Present work**	**other calculation**
	B3	0		0.0[a,b,c]		19.94[c]
				0.02[d]		16.0[d]
				0.5813[e]		
				0.753[c], 0.75[f]		34.0[c]
	B2	0	**0.08**		**16.5**	
				-0.354[g], -0.18[h],		23.4[g]
				-0.160[i], -0.118[g]		
				0.00[i], 0.03[h]		
						21.0[j]
				0.26[d], 0.694[g]		33.0[d], 31.0[g]
				0.711[g]		26.1[g]
				0.772[i], 0.805[g]		34.0[g]
InN	B1	0		0.0573[e], 0.22[a], 0.372[k]		9.4[e]
				0.6153 [e]		64.7[e]
				0.6887 [e]		
				0.7438 [e]		44.7[e]
	B3-B1	10.0		0.00[a], 0.081[l]		
		10.5[k]				
		11.84[m]				
	B2-B1	10.0	**0.28**		**33.0**	
		10.2		0.4[n]		18.0[n]
		10.86[m]				

		11.1		0.75[k]		24.9[k]
		13.0		0.1803[e], 1.3249[e], 1.4571[e]		
		16.0				22.0[o]
		21.6		1.66[d]		41.0[d]

[a]Plane wave self-consistent method with GGA-PBE (Ref. 1).

[b]FP-LAPW method with MBJLDA (modified Becke-Johnson exchange potential+LDA) (Ref. 2).

[c]FPLAPW method with LDA (Ref. 3).

[d]Self-consistent LMTO method with LDA-ASA (Ref. 4).

[e]PAW method with HSE06, GW, and GGA, respectively (Ref. 5).

[f]PW-PP method with LDA+ HGH (Ref. 6).

[g]PAW method with PBE, HSE06, G_0W_0(HSE06), $scGW_0$, G_0W_0(PBE), and GGA, respectively (Ref. 7).

[h]PAW method with LDA+U (Ref. 8).

[i]PAW method with GGA, GGA+U, and HSE, respectively (Ref. 9).

[j]LAPW method with LDA (Ref. 10).

[k]Troullier-Martins pseudopotentials, DFT-LDA (Ref. 11).

[l]FP-LAPW method with GGA-EV (Ref. 12).

[m]DFT with both LDA and GGA (Ref. 13).

[n]Plane wave pseudopotential with LDA (Ref. 14).

[o]Plane wave basis and with pseudopotentials, LDA+U (Ref. 15).

References

1 J. M. Panchal, M. Joshi, P. N. Gajjar, *Phase Transitions*, 2016, **89**, 1-27.

2 M. I. Ziane, Z. Bensaad, B. Labdelli, H. Bennacer, *Sensors Transducers*, 2014, **27**, 374-384.

3 S. Berrah, H. Abid, A. Boukortt, M. Sehil, *Turk J Phys.*, 2006, **30**, 513-518.

4 N. E. Christensen, I. Gorczyca, *Phys. Rev. B*, 1994, **50**, 4397-4415.

5 Alvarado, Andrew Michael, High-Pressure Properties of Several Narrow Band gap Semiconductors from First-Principles Calculations, 2016, UNLV *Theses, Dissertations, Professional Papers, and Capstones.* 2629.

6 S. Q. Wang, H. Q. Ye, *J. Phys.: Condens. Matt.*, 2002, **14**, 9579-9587.

7 Y. F. Duan, L. X. Qin, L. W. Shi, G. Tang, *Computational Materials Science*, 2015, **101,** 56-61.

8 A. Janotti, D. Segev, C. G. Van de Walle, *Phys. Rev. B*, 2006, **74**, 045202-1-9.

9 J. Kaczkowski, *Acta Physica Polonica*, 2012, **121**, 5-6.

10 S. H. Wei, A. Zunger, *Phys. Rev. B*, 1999, **60**, 5404-5411.

11 J. Serrano, A. Rubio, E. Hernández, A. Muñoz, A. Mujica, *Phys. Rev. B*, 2000, **62**, 16612-16623.

12 R. Ahmed, H. Akbarzadeh, Fazal-e-Aleem, *Phy. B*, 2005, **370**, 52-60.

13 S. Saib, N. Bouarissa, *Phys. B: Conden. Matt.*, 2007, **387**, 377-382.

14 W. X. Feng, S. X. Cui, H. Q. Hu, W. Zhao, *Phys. Status Solidi B*, 2010, **247**, 313-317.

15 J. M. Besson, L. Bellaich, K. Kunc, *Phys. Stat. Sol.* (*b*), 1996, **198**, 469-474.