

Supplementary Material to the manuscript  
**Comparative study of structural and electronic properties  
of GaSe and InSe polytypes**

by J. Srour, M. Badawi, F. El Haj Hassan and A. Postnikov :  
bibliography of experiments and previous calculations

TABLE I. Lattice parameters of GaSe from experiments

Phase	$a$ (Å)	$c$ (Å)	$\bar{c}$ (Å)	Ref.	Year
$\beta$	3.755	15.94	7.97	1	1961
$\gamma$	3.755	23.92	7.973	1	1961
$\varepsilon$	$3.755 \pm 0.002$	$15.946 \pm 0.003$	7.973	2	1971
$\delta$	3.755(3)	31.990(10)	7.998	3,4	1975
$\varepsilon$	$3.755 \pm 0.002$	$15.959 \pm 0.012$	7.980	5	1978
$\beta$	3.750(4)	15.995(7)	7.998	6	1988
$\beta$	$3.74 \pm 0.01$	$16.10 \pm 0.05$	8.05	7	1989
$\gamma$	$3.7 \pm 0.1$	$24.0 \pm 0.8$	8.0	7	1989
$\varepsilon$	$3.7 \pm 0.1$	$16.0 \pm 0.5$	8.0	7	1989
$\varepsilon$	3.743	15.919	7.960	8	1991
$\varepsilon$	3.753	15.91	7.96	9	2005
$\varepsilon$	3.7591	15.968	7.984	10	2007
$\varepsilon$	3.7384	16.0282	8.0141	11	2010

TABLE II. Optimized lattice parameters of GaSe from DFT calculations

Phase	$a$ (Å)	$c$ (Å)	$\bar{c}$ (Å)	Method / XC	Ref.	Year
$\epsilon$	3.724		7.839	DFPT / LDA	12	1998
$\epsilon$	3.720	15.620	7.810	WIEN2k / LDA	13	2006
$\beta$	3.83	16.29	8.145	WIEN2k / PBE	14	2009
$\beta$	3.80	16.17	8.085	VASP / PBE	14	2009
$\epsilon$	3.738	15.657	7.829	<i>abinit</i> / LDA	15	2010
$\epsilon$	3.662	15.587	7.794	<i>abinit</i> / LDA	16	2011
$\beta$	3.830	16.393	8.197	WIEN2k / PBE	17	2013
$\epsilon$	3.822	16.281	8.141	WIEN2k / PBE	17	2013
$\beta$ or $\epsilon$	3.751	15.948	7.974	VASP / PBE+D2	18	2013
$\epsilon$	3.738	15.657	7.829	Quant.Espr. / LDA	19	2013
$\epsilon$	3.839	17.151	8.576	Quant.Espr. / PBE	19	2013
$\epsilon$	3.798	15.886	7.943	Quant.Espr. / vdW-DF2	19	2013
$\epsilon$	3.743	15.919	7.965	Quant.Espr. / PBE+D2	19	2013
$\epsilon$	3.711	15.67	7.835	CASTEP / LDA	20	2014
$\epsilon$	3.72	15.74	7.87	Quant.Espr. / LDA	21	2014

TABLE III. Lattice parameters of InSe from experiments

Phase	$a$ (Å)	$c$ (Å)	$\bar{c}$ (Å)	Ref.	Year
$\gamma$	4.00	24.85	8.283	22 <sup>a</sup>	1974
$\gamma$	4.00	25.32	8.44	23	1975
$\beta$	4.005(5)	16.640(4)	8.320	24	1979
$\gamma$	4.002(1)	24.946(6)	8.315	25	1980
$\gamma$	4.002(1)	24.946(6)	8.315	26	1981
$\beta$	$4.00 \pm 0.04$	$16.7 \pm 0.2$	8.35	27	1986
$\gamma$	$4.00 \pm 0.04$	$25.3 \pm 0.3$	8.43	27	1986
$\gamma$	4.002	24.946	8.315	28	2003
$\gamma$	4.002	24.961	8.32	29	2017

<sup>a</sup>This publication cites earlier works which we could not directly inspect:  $a=4.023$  Å,  $c=25.05$  Å for  $\gamma$  from Schubert+Dörre+Gunzel, *Naturw.***41**, 448 (1954) and  $a=4.05$  Å,  $c=16.93$  Å for hexagonal phase ( $\beta?$ ) from Semiletov, *Kristallogr.* (1958), p.2988.

TABLE IV. Optimized lattice parameters of InSe from DFT calculations

Phase	$a$ (Å)	$c$ (Å)	$\bar{c}$ (Å)	Method / XC	Ref.	Year
$\gamma$	4.01	24.56	8.187	WIEN97 / LDA	30	2002
$\gamma$	4.02	24.42	8.140	PW( $E$ ) / LDA	30	2002
$\gamma$	3.99	23.59	7.863	PW( $p$ ) / LDA	30	2002
$\gamma$	4.01	23.93	7.98	SIESTA / LDA	30	2002
$\gamma$	3.953	24.138	8.046	<i>abinit</i> / LDA	31	2004
$\beta$	3.97	16.45	8.225	Quant.Espr. / LDA	21	2014
$\gamma$	3.99	25.31	8.437	VASP / PBE+D2	32	2015
$\gamma$	3.95	16.92	8.46	VASP / PBE+D2	32	2015
$\beta$	4.029	17.615	8.808	WIEN2k / PBE	33	2016
$\epsilon$	4.036	16.70	8.35	WIEN2k / PBE	33	2016

TABLE V. Band gap values  $E_g$  in GaSe from experiments and GW calculations

Phase	direct/indirect	$E_g$ (eV)	comment	Ref.	Year
$\beta$	direct	$2.169 \pm 0.002$		34	1969
$(\gamma, \varepsilon)$	direct	$2.120 \pm 0.002$		34	1969
$\beta$	indirect	2.117		34	1969
$(\gamma, \varepsilon)$	indirect	2.065		34	1969
$\beta$	direct	2.050	exciton peak	35	1975
$\delta$	direct	2.026	exciton peak	35	1975
$\varepsilon$	direct	2.004	exciton peak	35	1975
$(\gamma, \varepsilon)$	direct	2.0196		36	1989
$(\gamma, \varepsilon)$	indirect	2.010		36	1989
$\varepsilon$	indirect	1.995		37	2006
$\varepsilon$	direct	2.020	at 300 K	37	2006
$\varepsilon$	direct	2.34	GW	16	2011
$\varepsilon$	direct	1.75	GW ( $\Gamma-\Gamma$ )	16	2011
$\varepsilon$	direct	1.99	GW ( $M-\Gamma$ )	16	2011
$\varepsilon$	direct	1.93	$G_0W_0$	38	2014
$\varepsilon$	direct	2.11	$GW_0$	38	2014

 TABLE VI. Band gap values  $E_g$  in InSe from experiments and GW calculations

Phase	direct/indirect	$E_g$ (eV)	comment	Ref.	Year
$\gamma$	direct	1.263	(at 293 K)	39	1978
$\gamma$	direct	1.3525	(at 1.6 K)	39	1978
$\gamma$	direct	$\sim 1.336$	(at 10 K)	40	1992
$\gamma$	direct	1.24	from Fig. 4 in Ref.→	41	2001
$\gamma$	indirect	1.34	from Fig. 4 in Ref.→	41	2001
$\gamma$	direct	1.29		28	2003
$\gamma$	direct	1.3	VASP + GW	32	2015
$\beta$	direct	1.1	VASP + GW	32	2015

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