Tight binding parameters of AlP

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I. PARAMETERS OF UNSTRAINED INSB

Tight Binding model	sp3d5s*
Interaction range	First nearest neighbour (4 neighbours per atom)
Target bands	Hybrid functional calculations (HSE06) by VASP(v 5.2.3)
Date obtained	Aug 2014
Reference	
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Nemo5 Database	

TABLE I: Description of the parameters

sp3d5s* Tight Binding parameters of Si are given by table II. The band structure and DOS of InSb are shown in 1 respectively. The effective masses and important bandedges are compared in table III.

InSb	
a_0	$5.6307\mathring{A}$
E_{sc}	1.031374
E_{pc}	7.498503
E_{s*c}	21.639631
E_{dc}	15.860026
λ_c	0.106031
E_{sa}	−3.175259
E_{pa}	5.094555
E_{s*a}	16.945030
E_{da}	13.521720
λ_a	0.328949
$V_{s_c s_a \sigma}$	−1.409162
$V_{s*_c s*_a \sigma}$	−2.641797
$V_{s_c s*_a \sigma}$	−1.105832
$V_{s_c p_a \sigma}$	2.185100
$V_{s*_c p_a \sigma}$	1.709427
$V_{s_c d_a \sigma}$	−1.319977
$V_{s*_c d_a \sigma}$	−0.204016
$V_{p_c p_a \sigma}$	2.767821
$V_{p_c p_a \pi}$	−0.905487
$V_{p_c d_a \sigma}$	−0.661011
$V_{p_c d_a \pi}$	1.424111
$V_{d_c d_a \sigma}$	−0.939787
$V_{d_c d_a \pi}$	1.136142
$V_{d_c d_a \delta}$	−1.112910
$V_{s_a s*_c \sigma}$	−1.155545
$V_{s_a p_c \sigma}$	2.069040
$V_{s*_a p_c \sigma}$	1.700743
$V_{s_a d_c \sigma}$	−1.346939
$V_{s*_a d_c \sigma}$	−0.202736
$V_{p_a d_c \sigma}$	−0.684709
$V_{p_a d_c \pi}$	1.432133

TABLE II: Slater Koster type ETB parameters of bulk InSb. All presented parameters except for the lattice constants are in the unit of eV. The lattice constants are in Angstrom.

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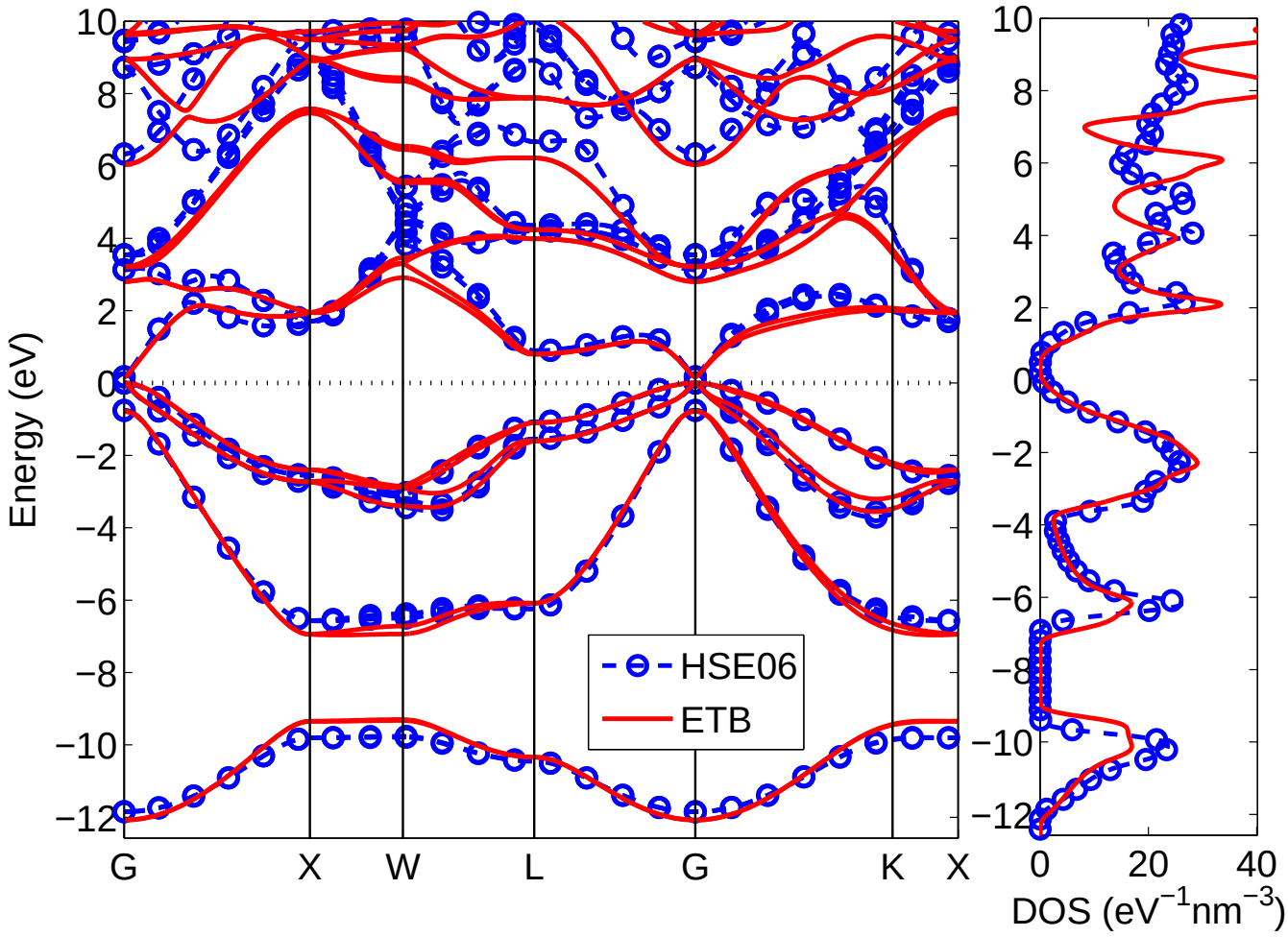

FIG. 1: Band structure and density of states of bulk InSb. ETB band structure agree with the HSE06 band structure (a), especially for bottom conduction bands (b) and top valence bands(c).

Target	DFT (eV)	TB (eV)	error(%)
$E_g(\Gamma)$	0.172585	0.161229	6.6
$E_g(X)$	1.566719	1.837321	17.3
$E_g(L)$	0.891456	0.798047	10.5
$Delta_{SO}$	0.754456	0.781855	3.6
$E_v(\Gamma)$	3.799433	3.808662	0.2
γ_1	39.017	31.810	18.469
γ_2	19.560	15.930	18.556
γ_3	16.938	13.755	18.794
m_{hh100}	0.245	0.300	22.484
m_{hh110}	0.452	0.542	19.963
m_{hh111}	0.609	0.734	20.365
m_{lh100}	0.012	0.015	23.328
m_{lh110}	0.013	0.016	20.569
m_{lh111}	0.012	0.014	24.109
m_{so100}	0.117	0.134	14.562
m_{so110}	0.117	0.134	14.305
m_{so111}	0.117	0.134	14.599
m_{c100}	0.011	0.014	28.072
m_{c110}	0.012	0.016	25.108
m_{c111}	0.011	0.014	28.942
m_{cXL}	0.877	1.149	30.910
m_{cXT}	0.219	0.317	44.531
m_{cLL}	1.685	1.933	14.751
m_{cLT}	0.096	0.134	39.564
m_{c2XT}	0.241	0.367	52.153

TABLE III: Targets comparison of bulk InSb. Critical band edges and effective masses at Γ, X and L from TB and HSE06 calculations are compared. The E_g and Δ_{SO} are in the unit of eV; effective masses are scaled by free electron mass m_0. The error column summarizes the discrepancies between HSE06 and TB results.