Tight binding parameters of InAs

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I. PARAMETERS OF UNSTRAINED INAS

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	
Authors	Yaohua P. Tan
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 InAs are shown in 1 respectively. The effective masses and important bandedges are compared in table III.

InAs	
a_0	$5.6307\mathring{A}$
E_{sc}	2.302580
E_{pc}	8.370285
E_{s*c}	24.012691
E_{dc}	16.373934
λ_c	0.106031
E_{sa}	−5.502749
E_{pa}	5.049144
E_{s*a}	22.668600
E_{da}	13.949303
λ_a	0.160931
$V_{s_c s_a \sigma}$	−1.481759
$V_{s*_c s*_a \sigma}$	−3.695365
$V_{s_c s*_a \sigma}$	−1.782697
$V_{s_c p_a \sigma}$	2.569215
$V_{s*_c p_a \sigma}$	2.238088
$V_{s_c d_a \sigma}$	−1.576994
$V_{s*_c d_a \sigma}$	−0.254846
$V_{p_c p_a \sigma}$	3.591088
$V_{p_c p_a \pi}$	−1.148472
$V_{p_c d_a \sigma}$	−0.337095
$V_{p_c d_a \pi}$	2.167329
$V_{d_c d_a \sigma}$	−0.871815
$V_{d_c d_a \pi}$	1.351395
$V_{d_c d_a \delta}$	−1.350150
$V_{s_a s*_c \sigma}$	−1.151180
$V_{s_a p_c \sigma}$	2.550779
$V_{s*_a p_c \sigma}$	2.287784
$V_{s_a d_c \sigma}$	−1.221846
$V_{s*_a d_c \sigma}$	−0.380596
$V_{p_a d_c \sigma}$	−0.913584
$V_{p_a d_c \pi}$	1.947015

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

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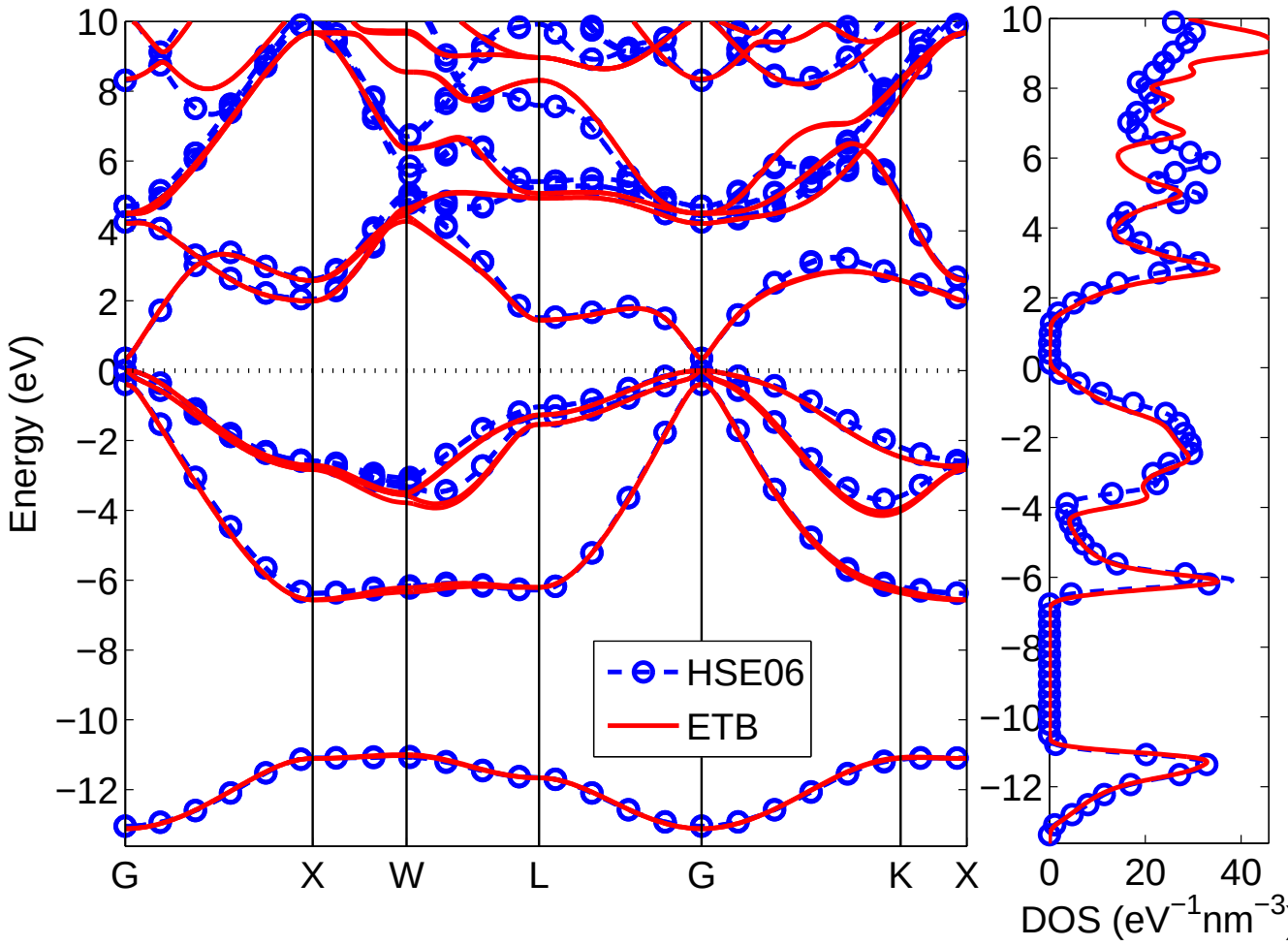

FIG. 1: Band structure and density of states of bulk InAs. ETB band structure agree with the HSE06 band structure (a), especially for bottom conduction bands (b) and top valence bands(c).

Target	DFT (eV)	TB (eV)	error(%)
$E_g(\Gamma)$	0.350726	0.347059	1.0
$E_g(X)$	2.052520	1.994117	2.8
$E_g(L)$	1.514575	1.445715	4.5
$Delta_{SO}$	0.391471	0.397117	1.4
$E_v(\Gamma)$	2.881317	2.903223	0.8
γ_1	19.027	18.986	0.214
γ_2	9.035	9.065	0.339
γ_3	8.011	7.997	0.174
m_{hh100}	0.344	0.358	3.905
m_{hh110}	0.625	0.636	1.874
m_{hh111}	0.835	0.848	1.525
m_{lh100}	0.026	0.026	0.003
m_{lh110}	0.026	0.026	0.020
m_{lh111}	0.025	0.025	0.276
m_{so100}	0.102	0.096	5.776
m_{so110}	0.102	0.096	5.780
m_{so111}	0.102	0.096	5.769
m_{c100}	0.022	0.022	0.252
m_{c110}	0.022	0.022	0.548
m_{c111}	0.022	0.022	0.185
m_{cXL}	1.458	1.404	3.712
m_{cXT}	0.232	0.211	9.072
m_{cLL}	1.904	1.927	1.208
m_{cLT}	0.114	0.123	7.493

TABLE III: Targets comparison of bulk InAs. 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.