Tight binding Parameters of unstrained GaSb

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I. PARAMETERS OF UNSTRAINED GASB

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 GaSb are shown in 1 respectively. The effective masses and important bandedges are compared in table III.

GaSb	
a_0	$5.6307\mathring{A}$
E_{sa}	1.698212
E_{pa}	8.275219
E_{s*a}	25.042527
E_{da}	14.803510
λ_a	0.024546
E_{sc}	−3.319697
E_{pc}	6.205015
E_{s*c}	22.926515
E_{dc}	14.595675
λ_c	0.345949
$V_{s_a s_c \sigma}$	−1.508819
$V_{s*_a s*_c \sigma}$	−3.909587
$V_{s_a s*_c \sigma}$	−1.367928
$V_{s_a p_c \sigma}$	2.714912
$V_{s*_a p_c \sigma}$	2.295490
$V_{s_a d_c \sigma}$	−1.900113
$V_{s*_a d_c \sigma}$	−0.259338
$V_{p_a p_c \sigma}$	3.548126
$V_{p_a p_c \pi}$	−1.286898
$V_{p_a d_c \sigma}$	−0.556841
$V_{p_a d_c \pi}$	2.032455
$V_{d_a d_c \sigma}$	−0.536190
$V_{d_a d_c \pi}$	1.321204
$V_{d_a d_c \delta}$	−1.276880
$V_{s_c s_a \sigma}$	−1.508819
$V_{s*_c s*_a \sigma}$	−3.909587
$V_{s_c s*_a \sigma}$	−1.333297
$V_{s_c p_a \sigma}$	2.565244
$V_{s*_c p_a \sigma}$	2.047945
$V_{s_c d_a \sigma}$	−1.338504
$V_{s*_c d_a \sigma}$	−0.193048
$V_{p_c p_a \sigma}$	3.548126
$V_{p_c p_a \pi}$	−1.286898
$V_{p_c d_a \sigma}$	−0.848827
$V_{p_c d_a \pi}$	2.101241
$V_{d_c d_a \sigma}$	−0.536190
$V_{d_c d_a \pi}$	1.321204
$V_{d_c d_a \delta}$	−1.276880

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

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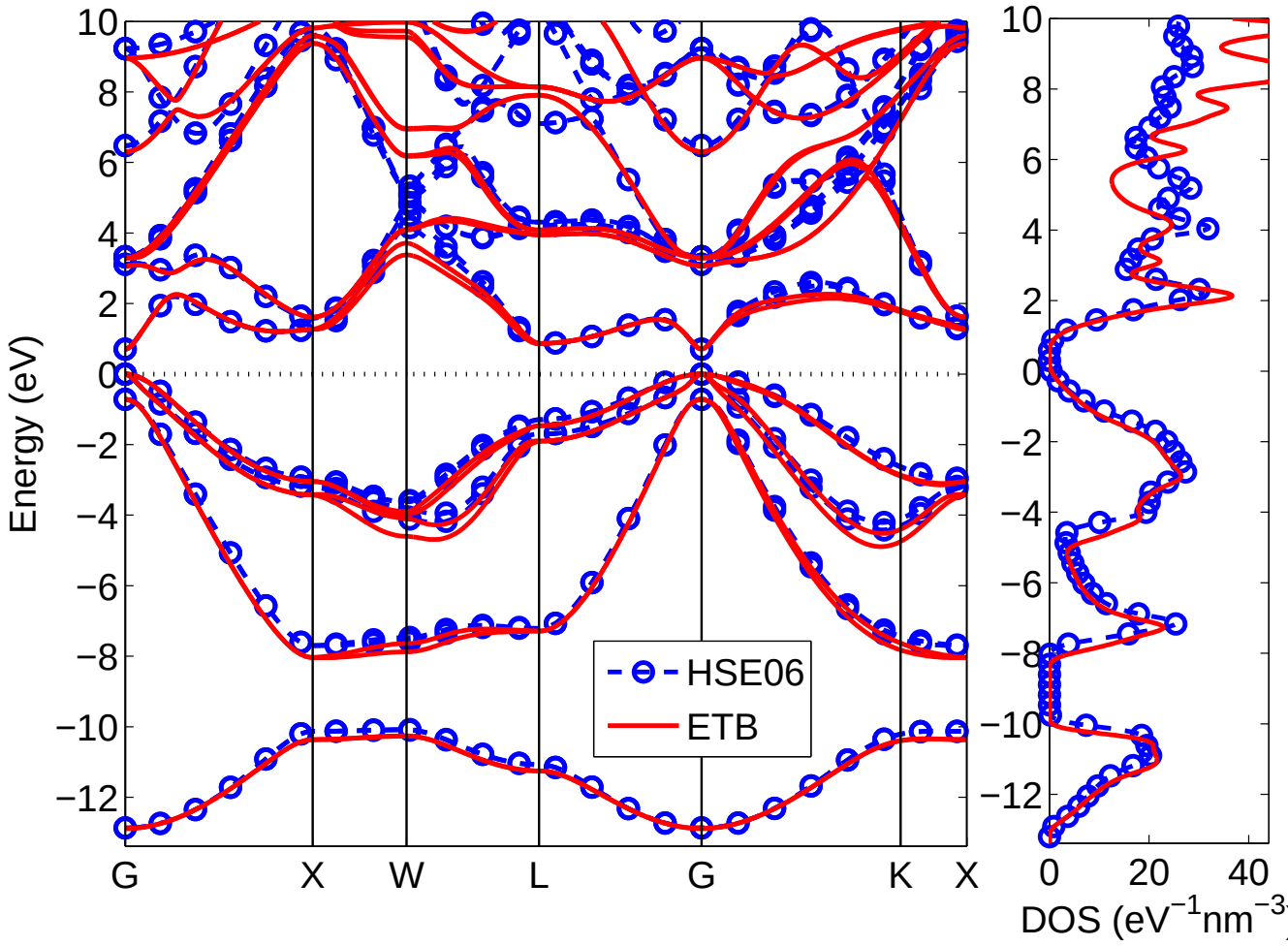

FIG. 1: Band structure and density of states of bulk GaSb. ETB band structure agree with the HSE06 band structure (a), especially for bottom conduction bands (b) and top valence bands(c).

Target	DFT (eV)	TB (eV)	error(%)
$E_g(\Gamma)$	0.707166	0.704523	0.4
$E_g(X)$	1.205590	1.203832	0.1
$E_g(L)$	0.865980	0.868921	0.3
$Delta_{SO}$	0.714750	0.722380	1.1
$E_v(\Gamma)$	3.855795	3.912224	1.5
γ_1	13.344	13.296	0.358
γ_2	5.142	5.220	1.528
γ_3	5.199	5.207	0.149
m_{hh100}	0.232	0.244	5.021
m_{hh110}	0.426	0.444	4.038
m_{hh111}	0.566	0.589	4.080
m_{lh100}	0.041	0.041	0.455
m_{lh110}	0.038	0.038	0.005
m_{lh111}	0.037	0.037	0.090
m_{so100}	0.137	0.127	7.538
m_{so110}	0.137	0.127	7.575
m_{so111}	0.137	0.127	7.569
m_{c100}	0.037	0.037	0.565
m_{c110}	0.037	0.037	0.544
m_{c111}	0.037	0.037	0.572
m_{cXL}	2.362	1.966	16.754
m_{cXT}	0.194	0.195	0.246
m_{cLL}	1.587	1.592	0.285
m_{cLT}	0.090	0.101	11.164
m_{c2XT}	0.229	0.233	1.414

TABLE III: Targets comparison of bulk GaSb. 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.