Tight binding analysis of Si and GaAs ultra thin bodies with subatomic resolution

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I. PARAMETERS OF UNSTRAINED GE

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	April 2015
Reference	
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Nemo5 Database	

TABLE I: Description of the parameters

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

Ge	
a_0	$5.6307\mathring{A}$
E_{sa}	-1.358375
E_{pa}	7.027423
E_{s*a}	26.480610
E_{da}	16.372930
λ_a	0.124125
$V_{s_a s_c \sigma}$	-1.728840
$V_{s*_a s*_c \sigma}$	-4.546952
$V_{s_a s*_c \sigma}$	-1.661106
$V_{s_a p_c \sigma}$	3.005207
$V_{s*_a p_c \sigma}$	2.664597
$V_{s_a d_c \sigma}$	-1.863717
$V_{s*_a d_c \sigma}$	-0.223341
$V_{p_a p_c \sigma}$	3.875101
$V_{p_a p_c \pi}$	-1.440461
$V_{p_a d_c \sigma}$	-0.706335
$V_{p_a d_c \pi}$	2.380497
$V_{d_a d_c \sigma}$	-1.093063
$V_{d_a d_c \pi}$	1.908442
$V_{d_a d_c \delta}$	-1.565951

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

Target	DFT (eV)	TB (eV)	error(%)
$E_g(\Gamma)$	0.755167	0.733727	2.8
$E_g(X)$	1.207427	0.894667	25.9
$E_g(L)$	0.709518	0.647106	8.8
$Delta_{SO}$	0.313002	0.309861	1.0
$E_v(\Gamma)$	3.503323	3.725295	6.3
m_{hh100}	0.212	0.209	1.641
m_{hh110}	1.508	1.608	6.625
m_{hh111}	0.496	0.497	0.119
m_{lh100}	0.212	0.209	1.641
m_{lh110}	0.212	0.209	1.675
m_{lh111}	0.496	0.497	0.119
m_{so100}	0.031	0.032	2.844
m_{so110}	0.028	0.029	1.780
m_{so111}	0.027	0.027	1.992
m_{c100}	0.033	0.034	3.196
m_{c110}	0.033	0.034	3.209
m_{c111}	0.033	0.034	3.201
m_{cXL}	0.838	0.793	5.443
m_{cXT}	0.188	0.188	0.045
m_{cLL}	1.572	1.855	18.003
m_{cLT}	0.081	0.096	17.280
m_{c2XT}	0.216	0.226	4.539

TABLE III: Targets comparison of bulk GaAs. 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.

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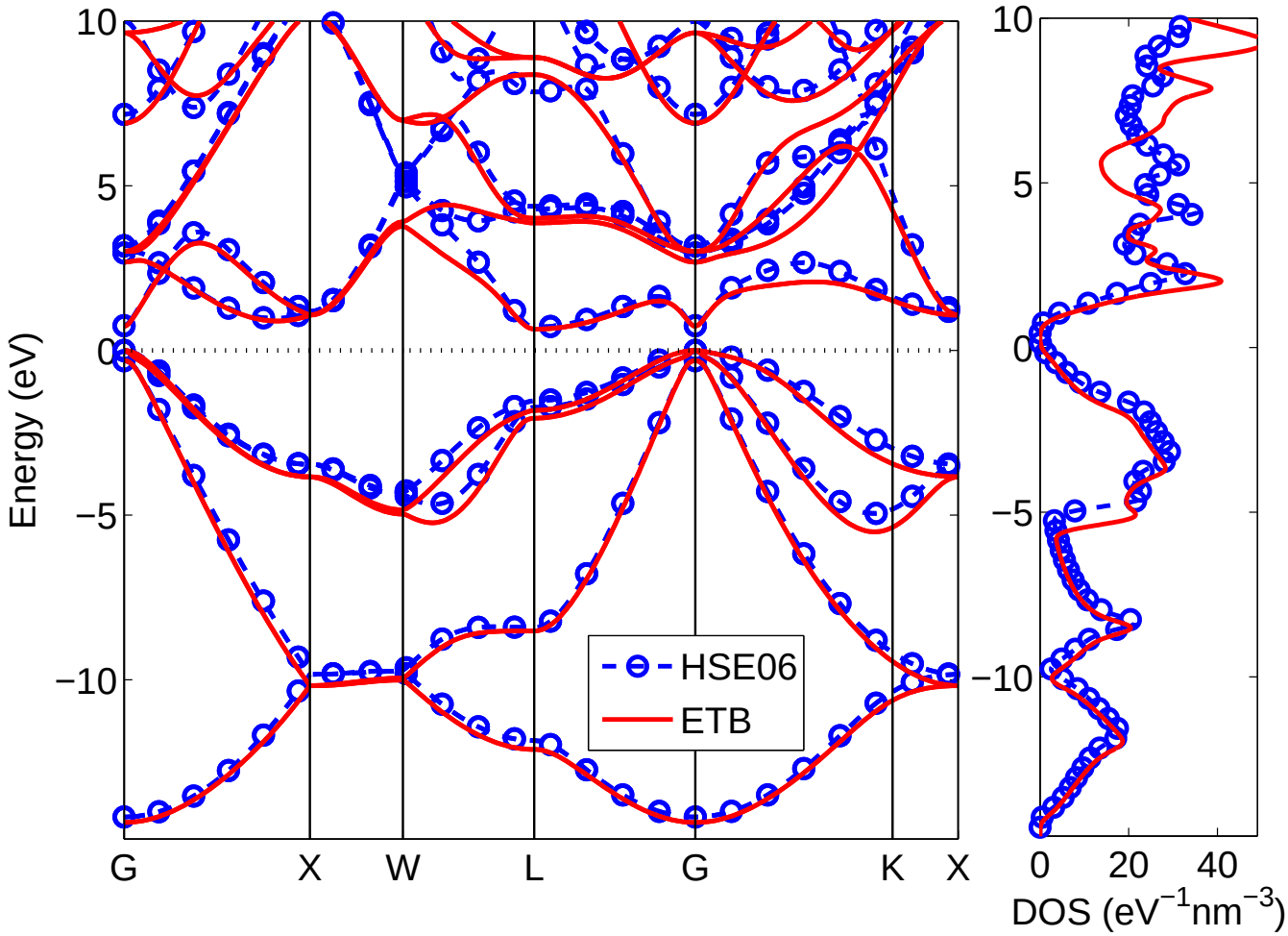

FIG. 1: Band structure and density of states of bulk Ge. ETB band structure agree with the HSE06 band structure (a), especially for bottom conduction bands (b) and top valence bands(c).