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

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I. PARAMETERS OF UNSTRAINED SI

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	Y. Tan,et al http://arxiv.org/abs/1503.04781 (2015)
Authors	Yaohua P. Tan
Nemo5 Database	param_HSE06_mapping

TABLE I: Description of the parameters

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

	Si
a_0	5.43Å
E_s	−2.803316
E_p	4.096984
E_{s^*}	25.163115
E_d	12.568228
Δ	0.021926
$V_{ss\sigma}$	−2.066560
$V_{s^*s^*\sigma}$	−4.733506
$V_{ss^*\sigma}$	−1.703630
$V_{sp\sigma}$	3.144266
$V_{s^*p\sigma}$	2.928749
$V_{sd\sigma}$	−2.131451
$V_{s^*d\sigma}$	−0.176671
$V_{pp\sigma}$	4.122363
$V_{pp\pi}$	−1.522175
$V_{pd\sigma}$	−1.127068
$V_{pd\pi}$	2.383978
$V_{dd\sigma}$	−1.408578
$V_{dd\pi}$	2.284472
$V_{dd\delta}$	−1.541821

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

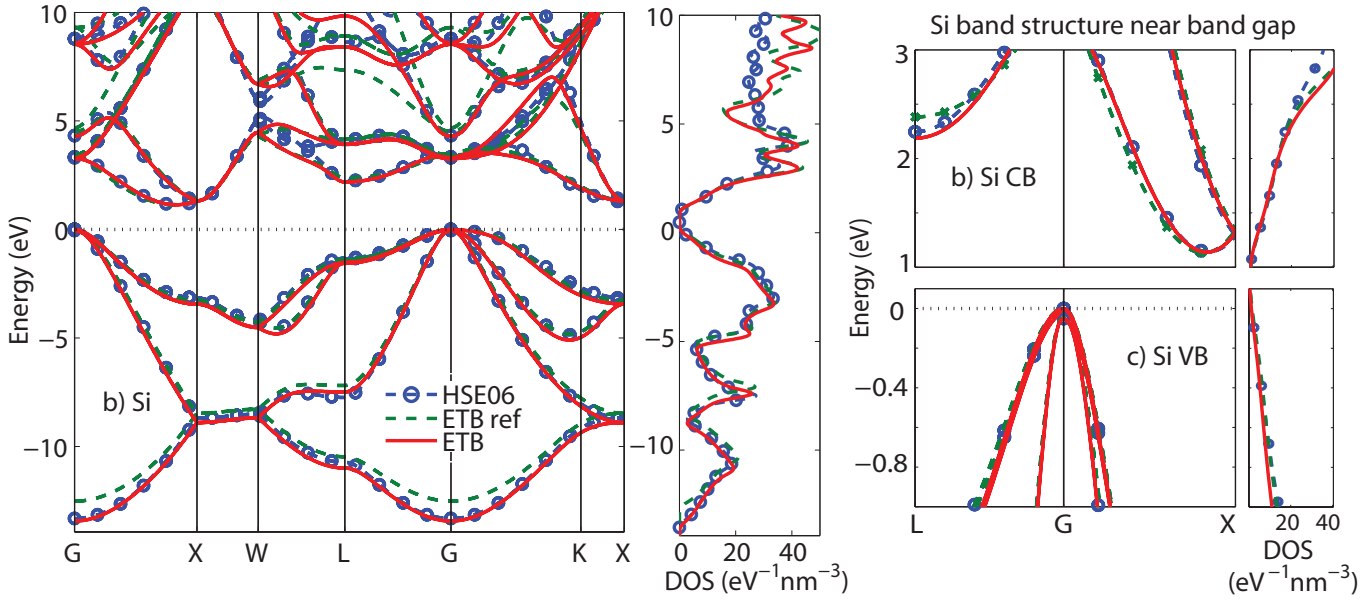

FIG. 1: Band structure and density of states of bulk Si. ETB band structure agree with the HSE06 band structure (a), especially for bottom conduction bands (b) and top valence bands(c).

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	Si			
targets	TB Ref	HSE06	TB	error (%)
$E_g(\Gamma)$	3.399	3.302	3.244	1.8
$E_g(X)$	1.131	1.142	1.139	0.2
$E_g(L)$	2.383	2.247	2.188	2.6
Δ_{SO}	0.047	0.051	0.052	0.8
m_{hh100}	0.299	0.281	0.282	0.097
m_{hh110}	0.633	0.566	0.572	0.977
m_{hh111}	0.796	0.704	0.714	1.433
m_{lh100}	0.232	0.206	0.204	1.001
m_{lh110}	0.165	0.151	0.149	0.937
m_{lh111}	0.156	0.143	0.142	0.927
m_{so100}	0.266	0.244	0.242	0.809
m_{so110}	0.266	0.244	0.242	0.795
m_{so111}	0.267	0.244	0.242	0.770
m_{cXl}	0.887	0.928	0.857	7.615
m_{cXt}	0.225	0.207	0.215	3.544

TABLE III: Targets comparison of bulk Si. Critical band edges and effective masses at Γ, X and L points by ETB 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.