

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

Yaohua P. Tan<sup>1,\*</sup>

<sup>1</sup>*School of Electrical and Computer Engineering, Network for Computational Nanotechnology,  
Purdue University, West Lafayette, Indiana, USA, 47906*

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## I. PARAMETERS OF UNSTRAINED ALAS

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

AIs	
$a_0$	5.6307Å
$E_{s_c}$	3.844665
$E_{p_c}$	9.171503
$E_{s^*c}$	27.975218
$E_{d_c}$	16.991734
$\lambda_c$	0.000000
$E_{s_a}$	-2.932564
$E_{p_a}$	7.882933
$E_{s^*a}$	27.897857
$E_{d_a}$	16.219579
$\lambda_a$	0.220931
$V_{s_c s_a \sigma}$	-1.884234
$V_{s^*c s^*a \sigma}$	-4.385365
$V_{s_c s^*a \sigma}$	-1.968153
$V_{s_c p_a \sigma}$	2.767410
$V_{s^*c p_a \sigma}$	2.568816
$V_{s_c d_a \sigma}$	-2.332389
$V_{s^*c d_a \sigma}$	-0.407474
$V_{p_c p_a \sigma}$	4.440040
$V_{p_c p_a \pi}$	-1.320667
$V_{p_c d_a \sigma}$	-1.373361
$V_{p_c d_a \pi}$	2.128562
$V_{d_c d_a \sigma}$	-1.406632
$V_{d_c d_a \pi}$	2.043294
$V_{d_c d_a \delta}$	-1.649027
$V_{s_a s_c \sigma}$	-1.884234
$V_{s^*a s^*c \sigma}$	-4.385365
$V_{s_a s^*c \sigma}$	-1.264778
$V_{s_a p_c \sigma}$	3.342574
$V_{s^*a p_c \sigma}$	2.386662
$V_{s_a d_c \sigma}$	-1.776396
$V_{s^*a d_c \sigma}$	-0.879660
$V_{p_a p_c \sigma}$	4.440040
$V_{p_a p_c \pi}$	-1.320667
$V_{p_a d_c \sigma}$	-1.141253
$V_{p_a d_c \pi}$	2.314171
$V_{d_a d_c \sigma}$	-1.406632
$V_{d_a d_c \pi}$	2.043294
$V_{d_a d_c \delta}$	-1.649027

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

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\* Electronic address: tyhua02@gmail.com

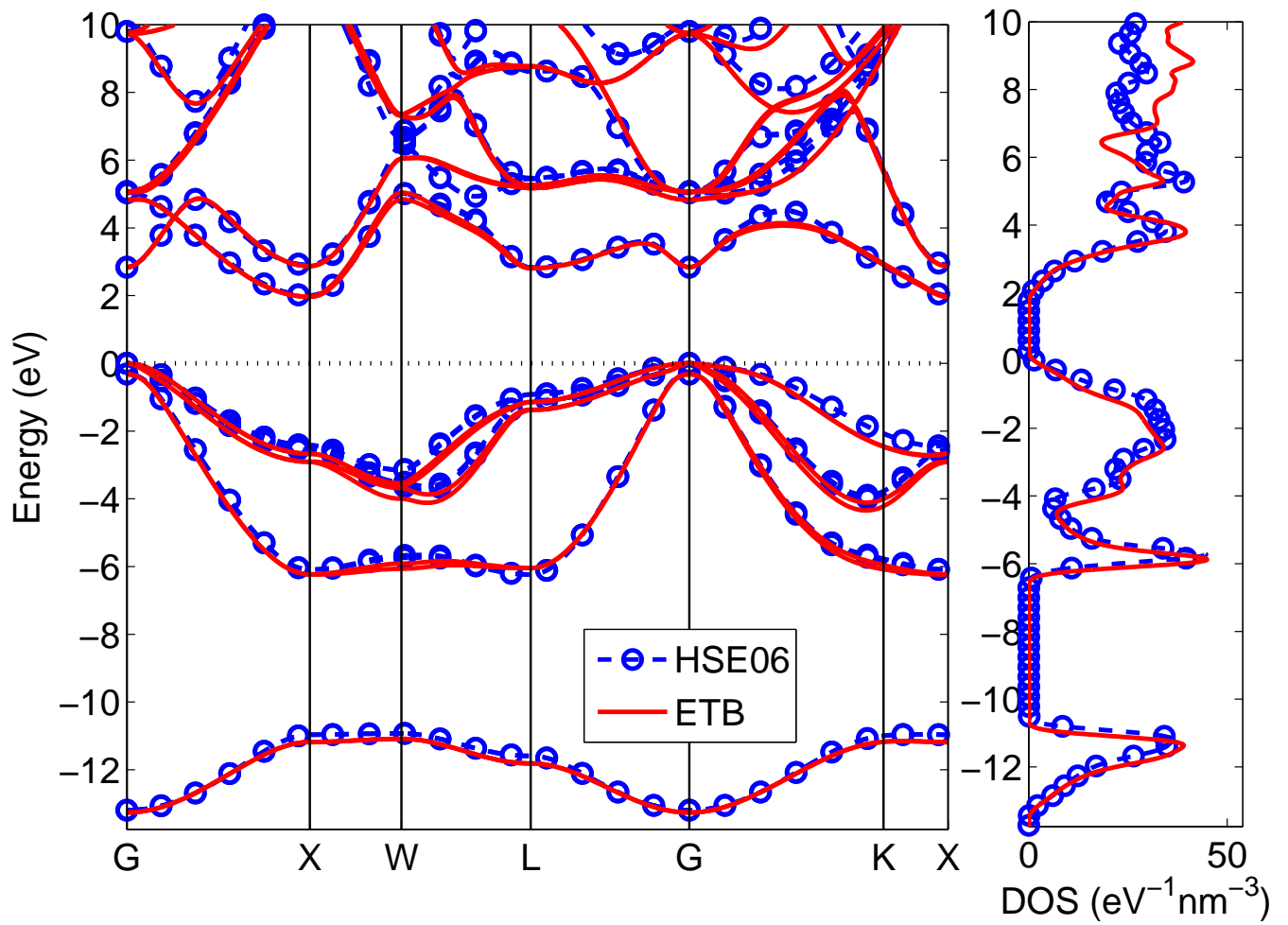


FIG. 1: Band structure and density of states of bulk AlAs. ETB band structure agree with the HSE06 band structure (a), especially for bottom conduction bands (b) and top valence bands(c).

Target	DFT (eV)	TB (eV)	error(%)
$E_g(\Gamma)$	4.186400	4.185930	0.0
$E_g(X)$	2.272698	2.261840	0.5
$E_g(L)$	3.632959	3.602002	0.9
$\Delta_{SO}$	0.064749	0.061687	4.7
$E_v(\Gamma)$	4.080850	4.132198	1.3
$\gamma_1$	2.831	3.000	5.963
$\gamma_2$	0.548	0.586	6.997
$\gamma_3$	0.931	0.991	6.438
$m_{hh100}$	0.508	0.482	5.151
$m_{hh110}$	0.998	0.944	5.358
$m_{hh111}$	1.273	1.224	3.812
$m_{th100}$	0.250	0.235	5.967
$m_{th110}$	0.201	0.190	5.686
$m_{th111}$	0.193	0.181	5.885
$m_{so100}$	0.343	0.319	6.881
$m_{so110}$	0.343	0.320	6.839
$m_{so111}$	0.343	0.320	6.895
$m_{c100}$	0.189	0.190	0.297
$m_{c110}$	0.189	0.190	0.285
$m_{c111}$	0.189	0.190	0.278
$m_{cXL}$	0.781	0.742	4.910
$m_{cXT}$	0.242	0.215	11.401
$m_{cLL}$	1.610	1.641	1.924
$m_{cLT}$	0.177	0.179	0.758
$m_{c2XT}$	0.236	0.251	6.484

TABLE III: Targets comparison of bulk AlAs. Critical band edges and effective masses at  $\Gamma$ ,  $X$  and  $L$  from TB and HSE06 calculations are compared. The  $E_g$  and  $\Delta_{SO}$  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.