Band offsets of $Al_xGa_{1-x}As$/GaAs heterojunction from atomistic first principles

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The properties of III-V compound semiconductors and their heterojunctions have been relentlessly investigated due to their wide-ranging applications in electronic and optoelectronic technologies. One of most important electronic property of heterojunctions is the band offset which describes the relative alignment of the electronic bands across the junction interface. Accurate determination of band offsets is critical for understanding quantum transport properties of the heterojuncton. For many III-V materials systems, the band offset has been carefully measured experimentally.[1]

On the other hand, theoretical calculations of band offset have proven to be a serious challenge. This is because first principles method of density function theory (DFT) with local-density approximation (LDA) and generalized gradient approximation (GGA) underestimates the band gap (E_g) of semiconductors. Without a correct calculation of E_g for individual semiconductors, the calculated band offset between two semiconductors can be problematic. Another theoretical difficulty is when there are impurities: the predicted physical results must be averaged over multitudes of impurity configurations which is extremely costly in computation.

Considerable theoretical efforts have been devoted in the literature to correctly predict E_g. Apart from the GW and hybrid functional methods, for calculating E_g of pure semiconductors, the recently proposed modified Becke Johnson (MBJ) semilocal exchange was shown to give quite accurate values for many compounds with "cheap" computational cost.[2] To deal with the prohibitively large computation required for calculating configuration average for doped semiconductors, one wishes to compute the averaged physical quantity in one-shot without individually computing each impurity configuration as in the super-cell approach. In this regard, a widely used technique is the coherent potential approximation (CPA)[3] as implemented in Korringa-Kohn-Rostoker or linear muffin-tin orbital (LMTO)[4] DFT methods. Very recently, Ref.[5] has combined CPA with MBJ and reported the calculation of E_g for the semiconductor $In_xGa_{1-x}N$, the results are in excellent agreement with the measured data for the entire range of $x = 0$ to 1.

In this work, we employ the CPA-MBJ first principles approach as implemented in the Nanodsim[6] software package to quantitatively calculate the band offsets of two semiconductors with impurity doping. In particular, we consider the most important heterojucntion, between GaAs and $Al_xGa_{1-x}As$. Our calculated E_g of $Al_xGa_{1-x}As$ for the entire x range, and the calculated band offsets of the heterojunctions, are all quantitatively and excellently compare with the experimental data.

References

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[6] For details of the NEGF-DFT code with CPA-MBJ, see Nanoacademic Technologies, http://nanoacademic.ca/.

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TABLE I

ENERGIES OF THE CONDUCTION BAND MINIMA AT THE Γ, X, AND L POINTS WITH RESPECT TO THE VALENCE MAXIMUM AT THE Γ POINT IN UNITS OF ELECTRON VOLT. THE COLUMN OF LDA^v WERE OBTAINED BY THE VASP ELECTRONIC PACKAGE USING LDA, OTHER RESULTS WERE BY NANODSIM WHICH IMPLEMENTS THE DFT WITHIN TB-LMTO APPROACH. THE LAST COLUMN ARE THE EXPERIMENTAL VALUES FROM REF.[1].

material	Eg	LDA^v	LDA	MBJ	Expt.[1]
GaAs	E_g^Γ	0.493	0.761	1.518	1.519
	E_g^X	1.334	1.346	1.960	1.981
	E_g^L	0.948	1.100	1.691	1.815
AlAs	E_g^Γ	2.014	2.300	3.099	3.099
	E_g^X	1.312	1.307	2.258	2.24
	E_g^L	2.086	2.191	2.835	2.46

TABLE II

USING THE CPA-MBJ APPROACH IN THE NANODSIM ELECTRONIC PACKAGE, THE FOLLOWING TABLE LISTS THE CALCULATED VBO AND CBO OF GAAS/AL_xGa_{1-x}AS HETEROJUNCTION.

x	0.1	0.2	0.3	0.4	0.5
VBO	0.070	0.114	0.167	0.222	0.280
CBO	0.050	0.145	0.238	0.276	0.230
x	0.6	0.7	0.8	0.9	1.0
VBO	0.337	0.397	0.459	0.532	0.593
CBO	0.210	0.190	0.167	0.161	0.148

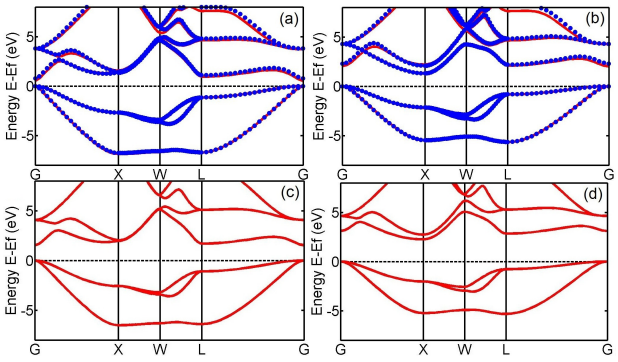

Fig. 1. (a,b) The band structures obtained with LDA: (a) for GaAs, (b) for AlAs. Red line is obtained by VASP, blue dots obtained by Nanodsim. A perfect agreement of the valence bands and a very good match of the conduction bands between these methods indicate that the TB-LMTO approach (Nanodsim) is quite accurate in calculating the physical properties of these materials. However, the band gaps were underestimated by LDA. (c,d) The band structures calculated with MBJ by Nanodsim: (c) for GaAs and (d) for AlAs. The MBJ band gaps are in good agreement with the experimental values at the Γ and X points, and within 7% for GaAs and 15% for AlAs to the experimental values at the L point, see Table I.

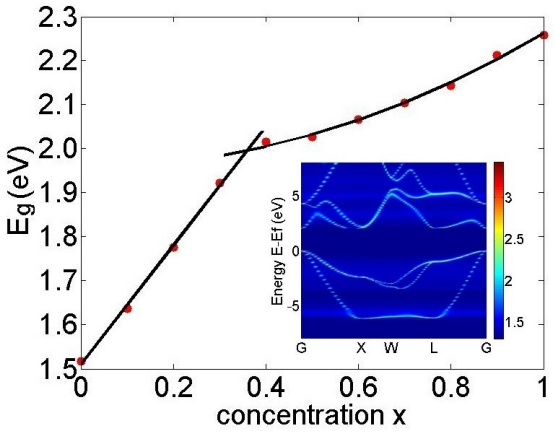

Fig. 2. The calculated band gaps of $Al_xGa_{1-x}As$ versus x by the CPA-MBJ approach. The two solid lines are fitting to the data in the two ranges of x. The alloy material changes from a direct-gap semiconductor to an indirect-gap one at a crossover point ($x \sim 0.36$) where the conduction band minima at Γ and X have the same energy value. Inset: the calculated DOS for the alloy $Al_{0.36}Ga_{0.64}As$ in logarithmic scale as a function of momentum k and energy E, revealing a broadened "band structure". The "conduction band" minima at Γ, X, and L points have essentially the same energy value for this alloy at $x \sim 0.36$.

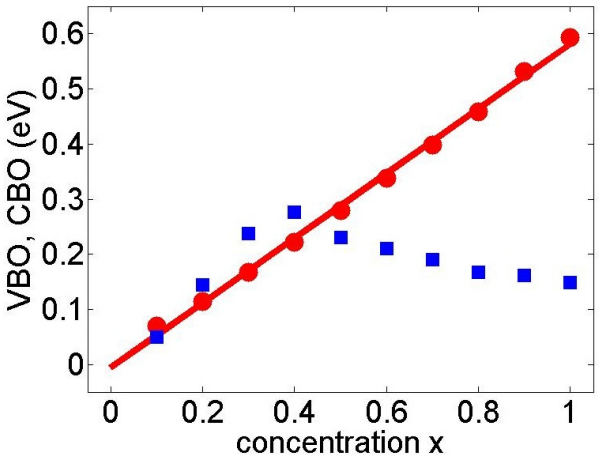

Fig. 3. Valence band offset (red dot) and conduction band offset (blue square) at different concentration x. The red line shows the linear fitting of the VBO, $VBO(x) \simeq 0.587x$ eV, which agrees reasonably with the experimental observation of $VBO(x) \simeq 0.55x$ eV. The GaAs/$Al_xGa_{1-x}As$ heterojunctions have the straddling type gap - the valence band maximum of GaAs is higher, while its conduction band minimum is lower.