Metal, Semiconductor, and Insulator properties calculated in VASP

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October 11, 2011

1 Introduction

VASP can be used to run various material simulations and molecular dynamics. Here, in the Keck Lab, we use VASP to run various material simulations in order to investigate new materials. VASP uses DFT with both LGA and GGA approximation-based pseudopotentials to calculate various material properties.

2 Metals

My calculations began with calculating bulk properties of solid copper. Using GGA potentials, I calculated the equilibrium lattice constant, equilibrium volume, ground state energy, and the bulk modulus for the three cubic lattices, as well as the diamond structure (FCC with a 2-atom basis).

Lattice Type	a_0	V_0	E_0	Bulk Modulus, β
Diamond	5.36 Å	38.50 Å^3	-2.73eV	23GPa
Simple Cubic	2.41 Å	14.07 Å^3	-3.28eV	112GPa
Body-Centered Cubic	2.89 Å	12.07 Å^3	-3.70eV	129GPa
Face-Centered Cubic	3.64 Å	12.06 Å^3	-3.73eV	166GPa
Experimental (FCC)	3.61 Å	11.76 Å^3	N/A	137GPa
DFT Reference[1]	3.52 Å	10.90 Å^3	N/A	190GPa

Because the BCC and FCC energies are so close, it seems that both BCC and FCC states might be equilibrium states for Cu.

3   Semiconductors

When looking at GaAs and trying to reproduce the band structure, amongst other equilibrium quantities, I ran into an interesting property of using GGA potentials with III-V semiconductors: the bands below the Fermi energy are generated perfectly, but the bands above the Fermi energy are much lower than expected. This makes the band gap ~ 0.1eV instead of the predicted 2.8eV. Kaxiras, in his paper, uses the LDA approximation, which reproduces a more accurate band structure. However, this approximation underestimates the equilibrium lattice constant and volume, and thus, over-approximates the bulk modulus. It also underestimates the equilibrium energy, E_0.

Quantity	GGA	LDA
a_0	5.76 $\mathring{A}$	5.63 $\mathring{A}$
V_0	47.90 $\mathring{A}^3$	44.60 $\mathring{A}^3$
E_0	-8.34eV	-9.65eV
Bulk Modulus, β	64GPa	82GPa

4   Insulators

Looking at an insulator provided a good contrast to the properties of metals and semiconductors. For this, I picked Si in a diamond lattice (which is the configuration for which it is an insulator). These are the results of calculations.

Lattice Type	a_0	V_0	E_0	Bulk Modulus, β
Diamond	5.47 $\mathring{A}$	40.92 $\mathring{A}^3$	-10.9eV	82GPa

5   Accuracy of DFT calculations

When using DFT to calculate material properties, the LDA and GGA approximations give a range of values which are either overstimates or underestimates. Experimental values always seem to fall in the range of these approximations, thus proving their validity.

References

[1] Mj Mehl and Da Papaconstantopoulos. Applications of a tight-binding total-energy method for transition and noble metals: Elastic constants, vacancies, and surfaces of monatomic metals. *Physical review. B, Condensed matter*, 54(7):4519–4530, August 1996.