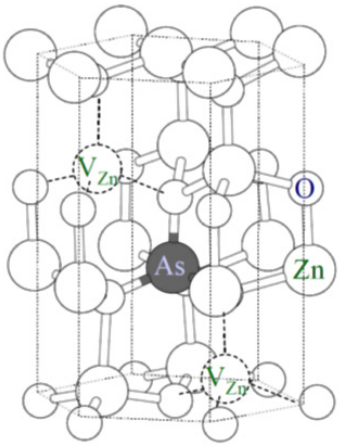
Homework 4: Computational Design of Materials

Due: December. 31, 2012

Formation energy and binding energy of defect complex in wide bandgap semiconductor ZnO

Natively grown ZnO is n-type, whereas p-type ZnO is very difficult to obtain. It is highly desirable to find a doping method to render ZnO into p-type. *Zn vacancy (V_{Zn}) is a native double acceptor*. Unfortunately, the vacancy has a very high formation energy (>2.2 eV in oxygen rich condition) and the transition energy level $V_{Zn}(0|-)$ is high (about 0.18 eV) too.

Co-doping technology can provide extra degree of freedom. Co-doping may be able to tailor V_{Zn} to yield more desirable energetic properties. One As_{Zn} and two V_{Zn} could form a new acceptor complex (As_{Zn}-$2V_{Zn}$). From the electronegativity of As (2.18 eV), it is similar to Zn (1.65 eV). In terms of atomic size, As (1.20 Å) is also similar to Zn (1.25 Å). Thus, it is expected that As should substitute Zn, instead of O. Indeed, Wahl *et al*. PRL **95**, 215503 (2005) confirmed As_{Zn} by channeling experiment.



Calculate the defect formation energy of the acceptor complex (As_{Zn}-$2V_{Zn}$) by using DFT and the defect structure shown on the left. Estimate the binding energy between As_{Zn} and V_{Zn} to verify one As_{Zn} and two V_{Zn} can bind strongly to form the acceptor complex (As_{Zn}-$2V_{Zn}$). Discuss the physics underlying your simulation result.