

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Quantum Monte Carlo models of substitutional point defects in zinc oxide and zinc selenide JAEHYUNG YU, ELIF ERTEKIN, Univ of Illinois - Urbana — Introducing dopants into semiconductors allows manipulation of electrical and optical properties, useful for applications such as optoelectronics and photovoltaics. While first principles quantitative descriptions of the defects properties in semiconductors are critical to understanding and engineering dopants in semiconductors, obtaining accurate descriptions has proven challenging in the past. Here we demonstrate the use of quantum Monte Carlo (QMC) methods to describing the properties of point defects in zinc oxide and zinc selenide. Due to its direct treatment of electron correlation, the QMC method is capable of accurate calculation of band gaps and defect behaviors. We describe the energetics and potential barrier to forming gallium DX-center defects according to QMC in zinc selenide, and compare the description to those of conventional and hybrid DFT. We also use QMC to determine the defect transition levels for nitrogen defects in zinc oxide, and show that QMC obtains descriptions that are in good agreement with GW and beyond-DFT approaches. Our results demonstrate the importance of accurate descriptions of electron correlation in the calculation of defect properties of semiconductors.

Jaehyung Yu
Univ of Illinois - Urbana

Date submitted: 13 Nov 2014

Electronic form version 1.4