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The Role of Vacancies on the Doping in Silicon Nanocrystals<sup>1</sup> JAE-HYEON EOM, TZU-LIANG CHAN, JAMES CHELIKOWSKY, University of Texas at Austin — We will present results for the effect of intrinsic defects (vacancies) on the doping of silicon nanocrystals by using first-principles calculations, *i.e.*, pseudopotentials in real space. We calculated the total energy of a B doped silicon nanocrystal as a function of the vacancy position and the nanocrystal size. We found that the most stable B site strongly depends not only on the cluster size, but also on the position of the vacancy. We also explored the evolution of the interaction between the vacancy and the B dopant by comparing the total energy for several nanocrystal sizes and configurations.

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