

Abstract Submitted
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Co-doping of Boron and Phosphorus in Silicon Nanoclusters JAE-HYEON EOM, TZU-LIANG CHAN, JAMES R. CHELIKOWSKY, University of Texas at Austin — The effect of cluster size on the interaction between impurity atoms is studied using the first-principles calculations, i.e. pseudopotentials in real space. We calculate the stable configurations of B and P co-doped silicon nanoclusters as a function of size. We evaluate the evolution of interactions between impurity atoms by comparing the stable configurations. The evolution of photoluminescence is discussed.

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