Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Tuning Electronic Structure of Si_{24} by Doping and Strain[1] JIAJUN LINGHU, LEI SHEN, Natl Univ of Singapore, MING YANG, Institute of Materials Research and Engineering, A*-STAR, YUANPING FENG[2], Natl Univ of Singapore
— Si24, a new allotrope of silicon with cmcm space group, has been synthesized recently and received much attention due to its quasi-direct band gap around 1.3 eV. Aiming to its potential application in solar cell device, in this study, we investigated the doping and strain effects on the electronic properties of Si_{24} using density-functional theory calculations with the hybrid functional. It is found that, Si_{24} can be easily doped as both p- and n-type semiconductors by III or V group elements. Among various potential dopants, B and P atoms are the most promising elements for the p-type and n-type doping in the Si_{24}, respectively, because of their relatively low formation and ionization energies. More importantly, the incorporation of these two dopants would not introduce impurity bands within the band gap of Si_{24}, but only cause a slightly narrowing of its band gap. Furthermore, through applying a small asymmetric compressive strain, the indirect band gap of pristine and doped Si_{24} can be tuned into the direct gap. It reveals the great potential in constructing novel Si_{24} based p-n junction which is highly desired for future industrial application in photovoltaic devices.

[1]Acknowledge to the High Performance Computing Resources at CA2DMGRC of NUS
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Date submitted: 10 Nov 2016 Electronic form version 1.4