# Theoretical study of vibrations and Raman spectra in pristine and P-doped Si nanocrystals

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Phonon confinement in Si nanostructures has been widely studied and size-dependent red-shifts as well as asymmetric broadening of Raman peaks have been commonly observed. However, a fully *ab initio* study of the Raman spectra in Si nanostructures has yet to be performed. Here, we investigate the vibrational modes and non-resonant Raman spectra of Si nanoclusters using density functional theory. Vibrational modes were calculated using the force constant method and non-resonant Raman spectra were evaluated within the Placzek approximation. We have reproduced the experimental Raman peak shifts and demonstrated that Raman spectra in Si nanocrystals are highly sensitive to the introduction of dopants.