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Raman spectra calculations for nanostructures using *ab initio* real-space methods[1] N. SCOTT BOBBITT, JAMES R. CHELIKOWSKY, University of Texas at Austin — We use a real-space pseudopotential method within density functional theory to calculate Raman spectra for Si nanocrystals. We examine the effects of quantum confinement and the presence of impurities, including dopant concentration and location of dopant within the nanocrystal. The ability to predict the effects of dopant concentration and location on a Raman spectrum from first principles suggests that this calculation technique could be coupled with spectroscopic experiments to identify the size and nature of doped nanocrystals.

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