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Ab initio calculations of surface effects on Raman spectra of BP-codoped Si nanocrystals[1] JOSHUA C. NEITZEL, JAMES R. CHELIKOWSKY, University of Texas at Austin — We use a real-space pseudopotential method implemented within density functional theory to calculate Raman spectra for B-doped, P-doped, and (B,P)-co-doped Si nanocrystals. We consider the role of dopant location, bonding structure, and nanocrystal size on these spectra. We find that features of the Raman spectra can be correlated with the dopant structure.

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