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**Raman spectra calculations for Si-Ge core-shell nanocrystals using *ab initio* real-space methods**[1] N. SCOTT BOBBITT, JAMES R. CHELIKOWSKY, Univ of Texas, Austin — We use a real-space pseudopotential method within density functional theory to calculate Raman spectra for Si-Ge core-shell nanocrystals. We examine the lattice strain induced by the interface of the core and the shell. We calculate how this strain affects the vibrational modes and Raman spectra. We also find that the relative size of the Si and Ge peaks in the Raman spectrum is proportional to the size of the Si core and Ge shell regions, which suggests that Raman spectroscopy can be used to experimentally determine the relative size of the core and the outer shell in these nanocrystals.

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N. Scott Bobbitt
Univ of Texas, Austin

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