

Abstract Submitted
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Raman spectra calculations for nanostructures using *ab initio* real-space methods¹ N. SCOTT BOBBITT, JAMES R. CHELIKOWSKY, The 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 both substitutional and interstitial impurities, such as lithium. The ability to predict the effects of dopant 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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Prefer Oral Session
 Prefer Poster Session

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