

August 11-14th at the Crowne Plaza Hotel in downtown Knoxville, TN



Contribution ID: 4

Type: **Poster Only**

Modeling the coupling between phonons and crystal electric fields

Vibronic states are frequently observed in neutron scattering when excited crystal electric field (CEF) levels and phonons are in the same energy range. Typically this coupling is modeled phenomenologically. Here we successfully model the phonon-CEF coupling from first principles using density functional theory and an electrostatic point charge model. We find we are able to account for the observed spectroscopic broadening in several Ce materials, and account for mysterious extra modes found at high energies.

Topical Area

Hard matter: quantum, electronic, semiconducting materials

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