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Electronic and vibrational properties of the $Na_{16}Rb_8Si_{136}$ and $K_{16}Rb_8Si_{136}$ clathrates KOUSHIK BISWAS, CHARLES W. MYLES, Department of Physics, Texas Tech University — We have studied the electronic and vibrational properties of the $Na_{16}Rb_8Si_{136}$ and $K_{16}Rb_8Si_{136}$ clathrates, using the local density approximation. In qualitative agreement with the rigid-band model, the electronic band structures display no major modifications due to inclusion of the alkali metal guests. However, the electronic densities of states show two sharply peaked structures and a dip near the Fermi level. This feature may help to qualitatively explain the temperature dependent Knight shift observed for the NMR active nuclei in $Na_{16}Rb_8Si_{136}$. Phonon dispersion curves show low frequency, localized "grattler" h modes for both clathrates. These modes may efficiently scatter the heat carrying host acoustic phonons, potentially suppressing the lattice thermal conductivity. Based on the harmonic oscillator model and on our calculated rattler frequencies, we predict the isotropic mean square displacement amplitude (U_{iso}) of the various guests in these clathrates. Our predicted values of U_{iso} for Na and Rb in $Na_{16}Rb_8Si_{136}$ are found to be in good agreement with experiment.

Koushik Biswas
Department of Physics, Texas Tech University

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