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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, Lubbock TX 79409-1051 — We have studied the electronic and vibrational properties of the $Na_{16}Rb_8Si_{136}$and $K_{16}Rb_8Si_{136}$ clathrate compounds using first principles calculations. In qualitative agreement with the rigid-band model, the electronic band structures display no major modifications due to the inclusion of the alkali metal guests. The guest atom valence electrons occupy the Si_{136} conduction band states, resulting in a shift of the Fermi level into the conduction band of the "parent" Si_{136} framework. Unlike pristine Si_{136}, the electronic density of states of the filled clathrates 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 $Na_{16}Rb_8Si_{136}$.[1] The phonon dispersion curves for the filled clathrates reveal low frequency, localized "rattling" modes for the Na (or K) and Rb guest atoms. These flat rattler modes compress the highly dispersive host acoustic mode band width. As a consequence, the rattler modes may efficiently scatter the heat-carrying host acoustic phonons, potentially suppressing the lattice thermal conductivity.

[1]S. Latturner, B. B. Iversen, J. Sepa, V. Srdanov, and G. Stucky, Phys. Rev B 63, 125403 (2001).

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