

Electron-lattice interaction in $\text{Sm}_{1-x}\text{Y}_x\text{S}$ -like systems

Miguel Kiwi, Miguel Rivas, Jaime Rössler

Abstract

An Anderson-like Hamiltonian, which describes a cluster of a rare earth (Sm or Y) cation surrounded by six S anions, is used to model the electron-lattice interaction in mixed-valence systems. Coupling between the electronic and phononic variables is introduced, and two different phonon modes are considered: a breathing and an asymmetric one. The first, related to the ionic radius, is treated exactly. The asymmetric mode, which determines the sd-f hybridization, is dealt with in the Born-Oppenheimer approximation. Experimental results are adequately accounted for by this simple model.