Electron-phonon coupling in mixed-valence systems

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The electron-phonon interaction in mixed-valence systems is modeled on the basis of an Anderson-like Hamiltonian that describes a cluster of one metallic rare-earth cation surrounded by six anions. Coupling between the electronic and phononic variables is introduced, keeping two different phonon modes: a breathing and an asymmetric mode. 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. A variety of experimental results are adequately accounted for by this simple model, like the anomalous thermal expansion, the Debye-Waller factor, the phonon softening and broadening, and the charge-distance correlation.