

The Role of Lattice Vibrations in the Energy Landscape of Materials

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Alexandra (“Alex”) Navrotsky has been a pioneer in determining the factors that influence the stability of a material as a function of composition, pressure and temperature, not only at the “macro” scale, but also at the atomic scale. One of keys to making this link is the study of the material’s lattice vibrations. In this contribution, the role of lattice vibrations will be explored: from high-pressure phase equilibria to the stability of complex framework structures. Structural details determined from X-ray and neutron diffraction experiments are combined with results from vibrational spectroscopy, inelastic neutron scattering and lattice dynamic calculations. These studies provide important insights about the stability of a material, including an understanding of phase transitions, thermodynamic and elasticity anomalies, amorphization, etc. The influence and commonalities of strong rigid bonds and weaker, more flexible modes on the lattice dynamics and energetics of a range of framework structures – from feldspars to metal organic frameworks (MOFs) - will be discussed.