Barochemistry: Predictive Solid State Chemistry at Bond Energy Compression

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Modern advances in experimental and computational capabilities make realistic to develop new materials from design to discovery and development. The application of thermo-mechanical energy (by high pressures and temperatures) comparable to chemical bond energies in solids can contribute to this concept in unique ways, as it often converts simple molecular solids into novel three-dimensional network structures in high energy density states. Nitrogen is one of few systems unambiguously demonstrated the materials design to discovery concept via the theoretical prediction and subsequent discovery of cg-N above 110 GPa and 2000 K. Since then, numerous forms of extended phases have been predicted in nitrogen and other molecular systems at various pressures, which have yet been discovered and thereby stimulated the present study. In this lecture, I will present our recent discoveries of novel extended phases in a few simple molecular systems including N2 and CO2 and discuss about a few thermodynamic and kinetic principles associated with the pressure-induced electronic and structural changes, which can be investigated using synchrotron x-ray diffraction and inelastic x-ray Raman spectroscopy.