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High Energy Density Extended Solids

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Application of high pressure significantly alters the interatomic distance and, thus, the nature of intermolecular interaction, chemical bonding, molecular configuration, crystal structure, and stability of solid. With modern advances in high-pressure technologies, it is feasible to achieve a large (often up to a several-fold) compression of lattice, at which condition material can be easily forced into a new physical and chemical configuration. The high-pressure thus offers enhanced opportunities to discover new phases, both stable and metastable ones, and to tune novel properties in a wide-range of atomistic length scale, substantially greater than (often being several orders of) those achieved by other thermal (varying temperatures) and chemical (varying composition or making alloys) means. Over the past decade or two, a large number of new materials and novel phenomena have been discovered and predicted at extreme pressure-temperature conditions. Commonly observed under extreme conditions is the transformation of solids into more compact structures with itinerant electrons such as metallic and nonmetallic extended phases. Nonmolecular extended solids, particularly made of low Z elements such as hydrogen, carbon, nitrogen, oxygen, and fluorine, constitute a new class of high energy density solids, which can store a large sum of energy in their three-dimensional network structure ($\sim$ several eV/bond). Yet, a large cohesive energy of singly bonded (or sp3 hybridized) electrons gives rise to an extremely stiff lattice and novel electronic and optical properties. Broadly speaking, these molecular-to-nonmolecular transitions occur due to electron delocalization manifested as a rapid increase in electron kinetic energy at high density, but there are many outstanding questions as well regarding the exact nature of chemical bonding, phase stability, chemical mechanisms, and so on. These questions constitute fundamental chemistry unique to extreme pressure-temperature conditions, which will be discussed in this talk. Also presented are the future directions of high-pressure materials research in an emerging/complementary phase and time scales of dynamic and static high pressures.