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High-Pressure Induced New Phases and Properties in Typical Molecular Systems

TIAN CUI, State Key Lab of Superhard Materials, College of Physics, Jilin University

High pressure introduces new phases by the rearrangement of atoms and reconfigurations of electronic states in materials, often with new physical and chemical phenomena. Study of the new phases in typical molecular systems under high pressure is an interesting subject, such as energy storage materials of solid hydrogen and polymeric nitrogen, hydrogen-rich compound with high-Tc superconductivity under high pressure, high pressure induced metallization of hydrogen, etc. High-pressure structures and pressure-induced phase transitions in the typical molecular solids, such as solid iodine, CHBr3, N2/CN, HBr/HCl, hydrogen-rich compounds (H2S, ZrH2, AsH3, BaReH9, etc.), and group IVA hydrides (Si2H6, Ge2H6, Sn2H6, etc.) are investigated extensively by means of first-principles density functional theory and extensive prediction strategies (molecular dynamics simulation, simulated annealing, soft mode phase transition, random structure-searching method and evolutionary methodology etc.). The new structures and new properties derived from pressure-induced phase transitions in these typical molecular systems have been observed. It is showed that high pressure provides a path for producing new materials with new properties.