A Perspective on the Crystal Structures of high Pressure Elements and their Properties

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Recent advancements in instrumentations and improvements in structural refinement techniques have led to the characterization of many structures of solids at high pressures. Some of the structure types discovered is novel and not seen in solids under ambient conditions. Even for elemental solids, particularly at intermediate pressure regime, it was found that instead of adopting simple close-pack structures, open and complex structures, modulated structures or incommensurately modulated structures were often observed. These observations challenge the conventional concept of chemical bonding for solids and provide a fertile ground for the investigation of new physical phenomena in materials under high pressure. In this presentation, high pressure structures and transformations on specific elemental solids are illustrated and discussed. The purpose is to develop a conceptual framework for the description of the structures and the understanding of the nature of chemical bonding at high pressure. It is shown that the distinct electronic structure and structural features are related to other unusual properties such as superconductivity.

Keywords: high-pressure structures, electronic structure calculations, chemical bonding theory