Unusual Chemical Structures and Properties of Materials under Extreme Pressure Conditions

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Abstract:
Electronic structure calculation is an indispensable tool in the investigation of the structure and properties of materials under high pressure, particularly under conditions not easily amenable to experiment. There are several notable experimental discoveries, such as superconductivity in hydrides and metal-to-insulator transition in alkali elements that were motivated by results from computational predictions. These unexpected properties are consequences of changes in the crystal structure due to atomic orbital hybridizations. I will give a semi-quantitative scheme to explain pressure-induced structural transformations based on the conventional bonding concept. The structure-property relationship leading to the unusual superconductivity in superhydrides will be explained. Results of recent studies on the chemistry of minerals under the Earth's mantle conditions and a new method for locating the transitions state of structural transformations in crystalline solids will be presented.