

Materials under extreme conditions: Insight from Theory

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Structural response under extreme conditions is unique in each material and can be described by thermodynamic variables such as energy, temperature, and pressure. Along with temperature, pressure can change the chemical bonding of materials significantly, resulting in the formation of the new phases and/or the alteration of materials properties, such as electronic, mechanical, and magnetic properties. Recent advances in high pressure research during the last decades allow us to witness the synthesis of new materials that are known to be energetically unfavorable under ambient conditions, by manipulating the temperature and pressure to form less stable high pressure phases.

In this talk I will present a few interesting examples of the temperature and pressure induced structural transformations occurring in transition metals, oxides, and semiconducting materials. Martensitic transformations in solids through slipping and twinning, our discovery of a new iron-oxide compound, and a fascinating phenomenon of the electronic structural changes in semiconductor materials such as band-gap opening and closing under pressure will be discussed.