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Pressure Tuning of Matter to Unveil Novel 'Metastable' States

Abstract

The ongoing technological advances necessitate the discovery of new materials with exceptional functional properties to ensure superior efficiency, stability, and cost effectiveness. [1-4] The available options are inadequate as long as the search is limited to the stable ground states of materials. Alternatively, the oft-overlooked arena of 'metastable'phases promises us with limitless new possibilities. Indeed, the recent studies [4-7] suggest that the design and discovery of long-lived, thermodynamically metastable materials could potentially be the way forward for sustainable technologies. In my talk, I would present the experimental discovery of a few such metastable phases, namely 1) TiN2, which is a promising superhard material that contains unique nitrogen subunits with highly energetic N—N single bonds [6] 2) Ti3N4, which is the first semiconducting titanium nitride known to date.[7] 3) ZnxMn1-xO solid solution in metastable rocksalt phase [8] which is a promising photocatalyst for solar water splitting reaction and solar light harvesting applications. Although, these compounds possess positive enthalpies at room conditions, they were recovered in metastable form from high-pressure/temperature conditions. The strategy that was employed here by marrying first principles theoretical calculations to high-pressure synthetic techniques is a way forward towards sustainable development of novel metastable phases for real-life applications.

References:

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