Pressure Tuning of Matter to Unveil Novel 'Metastable' States

Seminario [1]
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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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Programma:

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