

## Microsymposium

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*Structure, bonding and dynamics under extreme conditions*

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Knowledge on the composition and structure of a material are essential to the understanding of the properties. Recent advances in structural prediction techniques from first-principles calculations have greatly enhanced the perspective on the large variety of new crystal types, particularly, under extreme conditions at high pressure and high temperature. The structural information helps to develop a new understanding on the change in chemical bonding in highly compressed solids. I will present the results and experience in the use of several structural prediction methods with examples drawn from recent studies on the outstanding problems in pressure-induced amorphization of SnI<sub>4</sub>, structural transformations, atomic dynamics and structural chemistry of simple elemental and molecular solids at high pressure and high temperature. Our results will highlight the successes, challenges and future development on the practical applications of these methods.

**Keywords:** Extreme conditions, Structure and chemical bonding, Atomic dynamics