

**[PO-D2]Poster Session 2**

Symposium D

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

**[P2-31]High pressure phase transition and structural stability of transition metal compounds**

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The lattice, charge, spin and other degrees of freedom in transition metal compounds couple to one another, giving these materials rich physics and properties. The extreme conditions of high pressure and high temperature provide a new way to create new structures that do not exist at ambient pressure, which has become an important way for the discovery of novel transition metal compounds. In recent years, important progress has been made in the theoretical prediction and high pressure synthesis of new structures. First, this work suggests a lot of new materials to be investigated by changing stoichiometry in phase diagrams. Taking the V-C binary system as an example, here we report the first-principles prediction of a new type of vanadium carbide,  $V_5C_3$ , which has an unprecedented stoichiometry in the V-C system. It is demonstrated that the new phase is mechanically stable, and is energetically favorable than known phases under high pressures. We believe that this work opens a door to materials design by changing stoichiometry. And the relationship between the crystal structure, electronic structure and physical properties are discussed. Secondly, the phase transition under high pressure will be analyzed to understand the structural stability of materials at high temperatures and high pressures, providing important theoretical basis for optimizing high-pressure synthesis conditions.