Physics & Astrophysics Colloquium

Theoretical Prediction of stable quaternary phases by Transition Metal Doping in orthorhombic-MoAlB Phase by the First-Principles Calculation: Is Doping always good?

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4:00 PM Friday, March 31, 2023, Room 211, Witmer Hall

Abstract: Declining abundance of nonrenewable fossil fuels has led to search for cost-effective, efficient, and clean energy generation methods such as fuel cells. Electrochemical splitting of water molecules generate hydrogen gas that can be harnessed as fuel in fuel cells. However, these electrochemical reactions are heavily dependent on expensive catalysts such as noble metals to proceed efficiently. Hence, tremendous research has been performed to seek alternatives for these expensive catalysts. Many materials such as transition metal dichalcogenides (TMDs), black phosphorus (BP), and heavy pnictogens have been reported as alternative materials due to abundance and promising performances. Recently, a family of layered materials known as MAX and MAB phases that have yet to be explored is also reported to be good catalyst for water splitting reaction. MAX and MAB phases, also known as ceramic nanolaminates, have been reported to possess excellent thermal and electrical conductivities, elastic stiffness, chemical and thermal-shock resistance, damage tolerance, and are readily machinable. Thus in the quest for finding cheap alternatives for expensive catalyst we explore into this thermodynamically stable, layered, MAB phases promising for various application. We herein explore the phase stability of ternary orthorhombic MoAlB phases by doping transition metal in place of Mo. A few of the predicted quaternary phases is found to be stable structure in terms of formation energy. Latter we try to characterize the property based on atomic properties of the atom and try to establish a trend for easy prediction of tuned MAB phases. The theoretically predicted stable MAB phases along with the structural preference is intended to guide experimental efforts and to give an insight into the stability for different crystal symmetries of quaternary MoAlB phases.

Refreshments at 3:30 PM in Witmer Hall, Room 215

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