Challenges and Opportunities in Computational Studies of 2D MXenes

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ABSTRACT

2D transition metal carbides and nitrides (MXenes) are a large family of materials with more than forty compositions synthesized since 2011, such as Ti_2CT_x, Nb_2CT_x, $Ti_3C_2T_x$, and $Mo_2Ti_2C_3T_x$. Some properties of 2D MXene flakes are high metallic electrical conductivity (up to 24,000 S/cm), high Young's modulus (~ 380 GPa for $Nb_4C_3T_x$), negative surface charges (zeta potential < -40mV) and hydrophilic surfaces. Many computational studies have investigated different aspects of MXenes, including the formation, stability, electronic structure, and some applications such as electrocatalysis. However, several areas have remained understudied. Because of MXenes' transition metal carbide core and their ability to wrap around metal and ceramic particles, MXenes have the potential to be used as additives in composites, but limited studies have looked into the interface of MXenes with metals or ceramics. Additionally, their 2D nature creates an opportunity to study transition metal carbides at the thinnest level possible (1-nm-thickness) and investigate the effect of defects, interfaces, grain boundaries, and extreme environment on their phase stability, transformation and performance. In this talk, I will present the latest compositional space of MXenes and discuss a few potential areas for computational studies of MXenes with a focus on mechanics, defects, interfaces, and phase transformation.