Seminar on Condensed Matter Theory

Group of Theoretical Physics at the Department of Condensend Matter Physics
of Charles University has a pleasure to invite you to attend the seminar

on 7 March 2019 at 13:00

at Faculty of Mathematics and Physics of Charles University, Ke Karlovu 5, 121 16 Praha 2

Seminar room F052

MSc. Zhongheng Fu

Beihang University (BUAA), Department of Material Science, Beijing, China; Technical University of Ostrava (VSB), IT4Innovations - National Supercomputing Center, Ostrava, Czech Republic

Mechanical and functional design of two-dimensional transition metal carbides

Two-dimensional transition metal carbides so-called MXenes, are considered to have broad applications in energy storage, electrocatalysis, water purification, electromagnetic shielding and other fields due to their excellent conductivity, hydrophilicity, and ion adsorption properties. In previous studies, researchers have focused on stability and electrochemical properties of ideal surface configurations, ignoring the effects of specific service conditions (e.g., strain, solution environment) despite the well known fact that the external environment can affect the properties of materials. Here, we explore the effects of surface functional groups and metal compositions of MXenes with respect to the thermodynamic stability, mechanical strengths, and electrochemical/topological properties. Number of properties exhibit a sudden trend change along the valence electron number of M. Under multiple loadings, the excellent electrochemical properties of MXenes remain, while the strain itself can modulate the migration path of Li to large extent. From our calculated results we conclude that the bare MXenes show better overall electrochemical properties, while the oxygen-functionalized MXenes show better mechanical properties. The above findings provide theoretical guidance for the future experimental design of MXenes with desirable properties.

For more information follow: theory.kfkl.cz/seminars.php
If you wish to receive regular updates on fothcoming seminars, contact T. Novotný (tno@karlov.mff.cuni.cz).