Usage Report for Fiscal Year 2016

Project Title: Electronic properties and applications of MAX phases and MXenes

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Recently, experimentalists succeeded to synthesize the two-dimension monolayers and multilayers of a particular family of transition metal carbides and nitrides with chemical composition of $M_{n+1}C_n$ and $M_{n+1}N_n$ (M is an early transition metal), which were named as MXenes. The MXenes are derived from exfoliation of the MAX phases --- $M_{n+1}AX_n$, where A is an element from groups 13-16 in the periodic table and X is carbon or nitrogen --- using the hydrofluoric acid. During the acid treatment, the A element is removed from the MAX phase and the surfaces of the obtained two-dimensional $M_{n+1}X_n$ are instantaneously terminated by F, OH and/or O groups. The MXenes have already found applications as energy storage materials.

In this study, I have deigned novel MAX phases and MXenes. By using a set of first-principles calculations, formation energies, elastic constants, and phonon spectra of the deigned compounds have been examined. My calculations show that many of the deigned compounds are locally stable and may be synthesized in near future.

Currently, I have focused on investigating the electronic properties of the deigned MAX phases and MXenes in detail. I have examined the effect of surface functionalization with F, OH, and O on electronic properties of MXenes. From my calculations, it is observed that without surface functionalization MXenes are metallic systems. However, upon surface functionalization, some of them turn into semiconducting. Also, I am collaborating with experimentalists to synthesize the predicted compounds in this study.