

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-Principles Molecular Dynamics Study on the Electric-double layer Capacitance of Water-MXene interfaces YASUNOBU ANDO, MINORU OTANI, CD-FMat, AIST — MXenes are a new, large family of layered materials synthesized from MAX phases by simple chemical treatments. Due to their enormous variations, MXenes have attracted great attention as promising candidates as anode materials for next-generation secondary batteries. Unfortunately, the specific capacitance of MXenes supercapacitors is lower than that of active-carbon ones. Theoretical investigation of the electric-double layer (EDL) at electrode interfaces is necessary to improve their capacitance. First-principles molecular dynamics (FPMD) simulation based on the density functional theory (DFT) is performed to estimate the EDL capacitance from a potential profile $V(z)$ and a charge distribution $q(z)$ induced by the ions at water- Ti_2CT_x ($T=\text{O}, \text{F}$) interfaces. Potential profiles $V(z)$ of both Ti_2CO_2 and Ti_2CF_2 decrease about 1.0 eV steeply in a region of only 3 Å from a Ti layer, which is the same profile at the platinum interfaces. On the other hand, induced charge distribution $q(z)$ depends on the species of surface termination. Induced electrons are introduced at Ti layers in the case of O surface termination. However, Ti_2CF_2 is not capable to store electrons at Ti layers because it is mono-valence anions. It indicates that effective surface-position of MXenes depends on the surface terminations. Our results are revealed that small induced charge leads the low EDL capacitance at MXene interfaces. This is because interface polarization due to strong interaction between water and Ti_2CT_x induces net charge. The surface net charge hinders the introduction of ion-induced charges.

Yasunobu ANDO
CD-FMat, AIST

Date submitted: 07 Nov 2016

Electronic form version 1.4