

Abstract Submitted  
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**Effect of Metal Ion Intercalation on the Structure of MXenes and its Impact on the Dynamics of Water in MXenes** NARESH OSTI, MICHEAL NAGUIB, Oak Ridge National Laboratory, Oak Ridge, TN, USA, ALIREZA OSTADHOSSEIN, ADRI VAN DUIN, The Pennsylvania State University, PA, USA, YURY GOGOTSI, Drexel University PA, USA, DAVID WESOLOWSKI, EUGENE MAMONTOV, Oak Ridge National Laboratory, Oak Ridge, TN, USA — MXenes are two-dimensional materials of sheet-like morphology invented as an alternative to graphene with a potential for energy applications. Because of the heterogeneous bonding between different species and the presence of surface functionalities, MXenes can be intercalated with different chemical species including metal ions and water. The presence of water in MXenes even at ambient conditions impacts their properties relevant to technical applications. Therefore, it is important to understand how intercalants change the structure of MXene and the behavior of water in these materials. Here, using different scattering techniques (x-ray and neutron), we found that intercalation of MXenes with potassium ion increases the c-lattice parameter, yielding a more homogeneous structure with higher water uptake compared to pristine MXenes. In the latter, inhomogeneous structure was observed, with most water residing between the MXenes stacks rather than in between the layers. We found a two orders of magnitude reduction in the diffusion coefficient of water resulting from potassium intercalation, which is in good agreement with the values predicted from ReaxFF simulation. Consequences of improved homogeneity on the water dynamics following metal ion intercalation will be discussed..

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