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Prediction and Characterization of MXenes for non-lithium ion battery anodes¹ PAUL KENT, YU XIE, HOULONG ZHUANG, Oak Ridge National Lab, YOHAN DALL'AGNESE, Universite Paul Sabatier, Toulouse, France, MICHAEL NAGUIB, Oak Ridge National Lab, MICHEL BARSOUM, YURY GOGOTSI, Drexel University — Rechargeable non-lithium-ion (Na⁺, K⁺, Mg²⁺, Ca²⁺, and Al³⁺) batteries have attracted great attention as emerging low-cost and high energy-density technologies for energy storage applications. However, their development is hindered by the limited choice of high-performance electrode materials. Building on our previous work for lithium-ion applications, here we show that MXene nanosheets, a class of two-dimensional transition-metal carbides, may serve as high-performing anodes for non-lithium-ion batteries by combined first-principles simulations and experimental measurements. Both O-terminated and bare MXenes are shown to be promising anode materials with high capacities and good rate capabilities, while bare MXenes show better performance. Our experiments clearly demonstrate the feasibility of Na- and K-ion intercalation into terminated MXenes. Moreover, stable multilayer adsorption is predicted for Mg and Al, which significantly increases their theoretical capacities. Our results provide insight into metal ion storage mechanisms on two-dimensional materials and also suggest a route to preparing bare MXene nanosheets.

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