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Interplay of H_2O and K^+ inside the channels of Mn_8O_{16} VIDUSHI SHARMA, MERZUK KALTAK, Stony Brook University, MARK HYBERTSEN, Brookhaven National Laboratory, MARIVI FERNANDEZ-SERRA, Stony Brook University — With the rapid growth in consumer electronics and electric vehicles, there is an increasing interest in developing high-density batteries, which requires investigation of robust electrode materials. One of these, α-MnO_2, is inexpensive and environmentally benign to manufacture. It consists of an arrangement of corner- and edge- shared MnO_6 octahedra forming a 2×2 tunnel structure, and belongs to a family of "octahedral molecular sieve structures" (OMS-2). Owing to the large tunnel cavity of OMS-2, cations such as K^+, Li^+, Ag^+, etc. as well as water molecules can be introduced into the 2×2 tunnel, thereby enabling us to tailor its chemical and physical properties. In this work, we focus on the incorporation of K^+ in the tunnel, which stabilizes α-MnO_2, in agreement with experiment. Our primary goal is to investigate the role of water in stabilizing the ions already present in a tunnel cavity, using first-principles density functional theory (DFT) calculations, including van der Waals interactions. We also analyze how the hydrogen-bond network competes with the ionic bonding of K^+ in the channel.

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