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Intercalating layered materials for energy storage

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Layered materials are widely used as energy-storage media in applications such as hydrogen storage and batteries. Computational approaches can provide valuable insights into the underlying storage mechanisms and shed light on strategies to improve materials performance. We have employed advanced hybrid functional calculations to study two types of intercalated layered materials: (1) hydrogen-intercalated MoS_2 and (2) sodium-intercalated MnO_2. Our goal is to elucidate intrinsic materials properties that affect energy storage.

We have studied the interactions of hydrogen with MoS_2 by exploring the equilibrium geometry, formation energy, and electronic behavior of interstitial H and H_2 molecules inside layered MoS_2 structures [1]. Interstitial H is identified to be a deep donor while H_2 molecules are electrically inactive and energetically more stable in MoS_2. To further shed light on the hydrogen-storage capacity of MoS_2, we have also explored the insertion energies of H_2 molecules as a function of hydrogen concentration and found that up to 13 H_2 molecules can be accommodated within the same interlayer spacing of an areal 3×3 supercell.

In the second part of the talk, I will discuss electronic and ionic conductions in layered $NaMnO_2$, a cathode material for sodium ion batteries. Free carriers are trapped to form small hole or electron polarons; hence, electronic conduction is through polaron hopping. Ionic conduction is in the form of sodium vacancy migration. Both electronic and ionic conduction can be significantly affected by the presence of point defects. We will discuss strategies, such as optimizing synthesis conditions and impurity doping, to improve electrical conduction and storage performance of $NaMnO_2$.

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[1] Z. Zhu, H. Peelaers, and C. G. Van de Walle, Phys. Rev. B 94, 085426 (2016).