

## Computational modeling of H/H+ migration in porous and layered materials

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Spatial confinement has strong impact on the chemical properties of molecules. The layers of *h*-BN, MoS<sub>2</sub>, and graphene are chemically very stable, if not inert, and the interlayer interactions impose pressure on the intercalated species. So, the chemistry in the interstitial space of a layered material is expected to be significantly different from the surface-adsorbed counterpart. Based on first-principles calculations combined with well-tempered metadynamics simulations, we report the chemical interactions and mobility of protons (H<sup>+</sup>) and protium (H) in the interstitial space of these layered materials. We show that both H<sup>+</sup> as well as H can be transported between the layers of *h*-BN and MoS<sub>2</sub> with low free energy barriers, while they are immobilized in graphite, in accordance with experimental observations.

In the case of anhydrous proton conducting porous materials like COFs and MOFs, the conductivity of the proton is mediated by guest molecules like imidazole, triazole etc. that operate at relatively high temperature [1,2]. Another type of materials that serve, as proton conductors, are the so-called materials with intrinsic proton conductivity. In these materials there is no need from a guest molecule to facilitate the proton conductivity [3]. In the second part of the talk we will discuss an opportunity to use a functionalized with acidic groups porous aromatic polymers as a materials with intrinsic proton conductivity.

In the last part of the talk the dynamics of a H+ from acidic zeolite OH – groups in the zeolite frameworks, containing transition metal clusters will be discussed. On the basis of ab-initio MD simulations we will show that that reversed spillover of hydrogen is a spontaneous process and modifies the properties of the active cite (transition metal cluster).

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