Spectroscopic properties of and water diffusion in mesoporous aluminosilicates via *ab initio*-based machine learning potentials

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Ordered mesoporous silica are widely utilized in industrial applications and also in the CRC1333 due to enhanced catalytic activity compared to the crystalline counterparts. Their electronic properties can be tailored with metal atoms such as aluminum atoms in ordered mesoporous aluminosilicates. Despite the importance, the effect of aluminum incorporation on the electronic and structural properties has not been fully understood from an atomistic perspective. We employ a machine learning potential (moment tensor potential) in combination with density-functional theory (DFT) to simulate structures and the infrared (IR) spectra of the aluminosilicates [1]. We use the melt quench process followed by the functionalization of the surface to obtain the atomistic structures. The peak frequencies of the simulated IR spectrum of the bulk aluminosilicates agree with experimental data and the Al atoms contribute to several frequency ranges. The theoretical pair distribution function (PDF) shows the presence of Al–O bonds with a length greater than the Si–O bonds, in agreement with the PDF derived from synchrotron X-ray powder diffraction. The incorporated Al atoms, which act as Lewis acid sites, are present at the mesopore surface as well as in the bulk. We study the diffusion of water in the mesopores and the density profile.

[1] J. Greif, Master's thesis, University of Stuttgart, 2023.