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Inelastic Neutron Scattering study of Brønsted acidity and water confinement in zeolites

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Zeolites, crystalline and microporous aluminosilicates, are one of the most important groups of functional materials. Zeolites are widely used as solid acid catalysts in petroleum refinery and petrochemical industries. Zeolites can be described as microcoporous polymorphs of quartz. Whilst quartz is SiO2, zeolites asmit the isomorphous substitution of Si by many tetrahedrally coordinated atom, typically Al (Si4+ à Al3+ + H+)
. In this way, the Si/Al ratio gives the
number of acid sites, but not their location and strength.The catalytic properties of a zeolite depend strongly on its acidity, and this in turns depends on: the total number of acid sites, their individual strength, and their individual location. These three factors are strongly correlated. Geometric parameters that are defined by the location of the acid site (i.e., bond angles and lengths around the acid site) make a remarkable contribution to the acid strength. It was found that the strong acid sites have the trend to be found in relatively small micropores.[1]
In the present work we study the zeolite LTA Si/Al= 40 (only one acid site per unit cell). The structure of LTA zeolite has the micropores consisting of large and small cavities. Inelastic neutron scattering (INS) has been used to study the acid sites of the LTA zeolite with different Si/Al ratios. There are two groups of bands: the first one found at 1050-1100 cm-1 that corresponds to the SiOH in-plane bending and another one found near 400-500 cm-1 which is attributed to the out-of-plane bending. These bending modes of the acid site are not no possible to measure with IR spectroscopy since these bands overlap with the strong bands from the zeolite framework. The combination of an extremely high quality of the samples and the sensitivity of the instrument allows to detect with high precision the acid sites of LTA Si/Al=40 and obtain information about its position. In order to fully understand the INS spectra we performed ab-initio calculations [2,3].
In addition the polar properties of zeolites can be nicely tuned by selecting the
appropriate chemical composition and concentration of structural defects in their frameworks. In the present study we were particularly interested about the mechanism of water adsorption on small pore zeolites and the influence of the polarity of the zeolite cavities in the clustering of water molecules when adsorbed in confined spaces, since there is controversy on the formation of hydroxonium cations when water is adsorbed on acid zeolites, and in case of hydroxonium formation, who many water molecules participate into the hydroxonium species. The simple framework of the chabazite (Fig. 1left) makes this zeolite and ideal candidate for the INS study of adsorbed molecules with theoretical approaches in order to provide a deep understanding on the influence of the polarity of zeolite on the clustering of adsorbed water [4].
References:[1] N. Katada et al., “J. Phys. Chem. C 2009, 113, 19208- 19217. [2] T. Lemishko et al., J. Phys. Chem. C 2016, 120, 24904−24909. [3] T. Lemishko et al., J. Phys. Chem. C 2018, 122, 11450−11454 . [4] M. Jimémez-Ruiz et al., manuscript in preparation.

Summary

Topic

1. Diffusive dynamics

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