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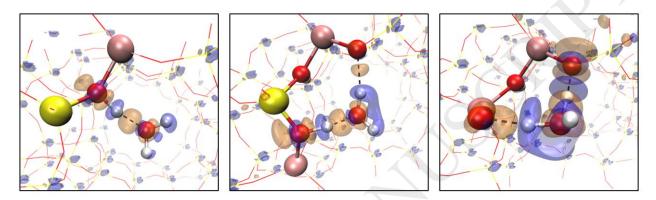
ACCEPTED MANUSCRIPT

Enhanced Chemical Activity and Wettability at Adjacent Brønsted Acid Sites in HZSM-5

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Graphical abstract



Highlights

- DFT calculations show enhanced adsorption of water in HZSM-5 when two acid sites are located in close proximity.
- The enhanced water adsorption results from increased polarization caused by the adjacent acid sites.
- A hydronium ion is formed when water interacts with adjacent acid sites.
- Hybrid functional calculations are essential for accurately describing the two acid sites located in the proximity.

The adjustable acid sites in zeolites and its well-defined pore structure allows for a fine-tuning of the catalytic performance. The activity and selectivity of several reactions have been shown to be dependent on the location and distribution of the acid sites in the zeolite. However, the underlying mechanisms responsible for this dependence remain to be explored. Here, we report density functional theory calculations, through which we investigate the impact of proximity of Download English Version:

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