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Sequential MD-QM approach to compute chemical properties of Brønsted amorphous aluminosilicate catalysts

Sequential MD-QM approach to compute chemical properties of Brønsted amorphous aluminosilicate catalysts Charles Rubirigi, Benoît Champagne NISM (Namur Institute of Structured Matter), University of Namur (UNamur), B-5000 Namur, Belgium charles.rubirigi@unamur.be

Amorphous silica-based materials are often used as support for catalysis experiments. The insertion of heteroelements (i.e., neither a silicon nor an oxygen atom) leads to the formation of Brønsted or Lewis acid sites.1 Despite their widespread use, these materials are still complex to characterize. Moreover, their amorphous nature further complicates the task.2 In this context, computing chemical properties with quantum chemical methods can bring insights into such materials. However, the large size of these systems implies the use of models to limit the computational effort.3

The present work shows a complete route to compute chemical properties on amorphous Brønsted aluminosilicate catalysts using a cluster approach. The amorphous network is generated using classical molecular dynamics via a thermal treatment called melt-and-quench. Particular attention is devoted to the catalyst shape and silanol coverage. The quality of the final amorphous network is assessed through geometrical analysis implying primitive ring size analysis. Density Functional Theory calculations are then performed on hemispheres extracted from the amorphous silica framework, where the central silicon atom is replaced by an aluminum atom. The impact of cluster size on the prediction of chemical properties is illustrated by deprotonation energies and chemical shift calculations. The influence of the XC functional on those quantities is also discussed.

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