Adsorption of Alanine and Phenylalanine on MFI-type Zeolite: DFT Calculations and Experimental Results

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Adsorption is a common unit operation in separation and purification of biotechnological products where chromatography steps can make up more than half the amount of the total purification costs. Quantum mechanics (QM) calculations may help to facilitate process design in a more cost efficient manner by predicting binding patterns to select adequate adsorbents. As a first step to investigate adsorption characteristics of biotechnological products such as proteins and peptides we want to explore the interaction of amino acids with zeolite surfaces, as potential of amino acid separation using zeolites was shown.

In this work the interaction of MFI-type zeolite MFI-27 (Al/Si=13) with Alanine and Phenylalanine is investigated by experimental adsorption isotherms accompanied by Isothermal Titration Calorimetry (ITC) at different pH values. The results are compared to corresponding QM data. For the QM calculations a T3-cluster is used as MFI-27 surface model. In order to model different pH values Alanine and Phenylalanine are applied in their protonated, zwitterionic and deprotonated state. Geometry optimisations and frequency analysis of all molecular structures are performed with Density Functional Theory (DFT) using the B3LYP functional. Calculated complex energies are corrected for BSSE and ZPE.

Obtained adsorption isotherms follow simple electrostatic considerations: high adsorption of Alanine and Phenylalanine on MFI-27 takes place at low pH values (near the pKa of the amino acids). Less adsorption occurs with an increased pH equalling the amino acids' isoelectric points. At the pH of the amico acids' pKb values adsorption is no longer observed.

These trends can be qualitatively correlated with the corresponding QM calculations. High binding energies are calculated for the protonated amino acids. Zwitterionic states lead to lower binding energies. The deprotonated amino acids do not show any binding affinity to MFI-27. Results from accompanying ITC measurements provide enthalpies of adsorption, which further help drawing assumptions on the binding characteristics of amino acids on MFI-27.