

This thesis is focused on theoretical study of influence of the silanol nest defects on the hydrolysis of zeolite Chabazite under harsh steaming conditions. The motivation of the thesis was a recent experiment proving that the silanol nest defect enhances the hydrolysis of a zeolite. The harsh steaming conditions have been chosen as some important technological processes involving zeolites require high temperatures and have water vapour present. The study was performed by using density functional theory calculations. To investigate the influence of the defect two models were used a reference pristine model and a defected model containing the silanol nest defect. The two models were pure siliceous Chabazite periodical models with supercell containing 36 and 35 Si tetrahedra respectively. A multi-step hydrolysis leading to detachment of a $\text{Si}(\text{OH})_4$ cluster from the zeolite, known as total desilication, was calculated for the two models. Multiple possible paths of the hydrolysis were discovered, compared and discussed on both models. Both the most favourable hydrolysis paths of the two model as well as their arithmetic means were compared. The experimentally set expectations that a silanol nest defect enhances the hydrolysis of the zeolite have been met.