



### Posudek školitele diplomové práce

**Author:** Tereza Benešová

**Title:** Mechanistic Insights into Reactive Zeolite-Water Interactions

**Opponent:** Mauricio Maldonado Domínguez, PhD.

**Supervisor:** Dr. Christopher J. Heard

Tereza Benešová started her work in our group during her Bachelor studies, in which she began to investigate the interaction of water with zeolitic materials via computational strategies, in particular, static density functional calculations of reaction energetics, binding modes and reaction barriers. In her diploma work, she has greatly expanded this area of interest in a number of important directions, including the discovery of novel reaction mechanisms, the effects of water loading, the role of temperature and dynamic effects on water-zeolite systems.

The primary aim of the study was to identify and enumerate the oxygen exchange mechanisms that lead to incorporation of water oxygens into the zeolite framework, without causing loss of framework integrity. This is an ongoing puzzle in the field of zeolites, and an important task for the better understanding of an industrially important class of materials. While non-reactive water-zeolite interactions have been well-studied for their relevance in catalytic applications of zeolites, such as in fluid catalytic cracking, reactive exchange processes are poorly understood. Hence, discovery of these mechanisms, and how they are affected by parameters such as water loading and choice of framework site, represents the theoretical basis for future collaborative work with leading experimental groups in the field, and an important advance in scientific knowledge.

In this thesis, this primary aim has been unambiguously achieved. Furthermore, via careful and systematic investigation, this thesis contains sufficient numerical data to allow for comparisons between hydrolysis and exchange processes, and between siliceous and aluminosilicate zeolites. All findings are in-line with current experimental understanding, and the work is in progress to being submitted to a peer-reviewed scientific journal.

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In order to achieve the scientific goals of the project, Bc Benešová was required to learn several new computational techniques, including alternative stationary point localization methods, *ab initio* molecular dynamics simulations, biased dynamics and free energy methods, such as thermodynamic integration. In each case, she was able to master the use of the methods, and showed great care in understanding the theoretical basis and the limitations of each method. She was able to work with independence and showed initiative in delving into the literature, double checking results, identifying alternative mechanisms and avoid gaps in datasets. She applied this independent and methodical approach to the writing of thesis, which is clear and well-structured.

Based on the above, I highly recommend the Diploma thesis for defence and recommend it for the highest classification of very good.

Dr. Christopher Heard  
Prague 07.09.22

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