DFT-Guided Insights into Zeolite-Based Catalysts for DeNOx-SCR Reaction

Matej Bubaš,[a,b] Matej Huš,[a,c] Nataša Novak Tušar[a,c] and Magdalena Jabłońska[d,e]

matej.bubas@ki.si

[a]*National Institute of Chemistry, Ljubljana, Slovenia*
[b]*Ruđer Bošković Institute, Zagreb, Croatia*
[c]*University of Nova Gorica, Nova Gorica, Slovenia*
[d]*Institute of Chemical Technology, Universität Leipzig, Leipzig, Germany*
[e]*University of Łódź, Faculty of Chemistry, Łódź, Poland*

Nitrogen oxides (NOx) are among the largest air pollutants and their abatement is a focus of intense ongoing research. One of the best ways of NOx abatement is through selective catalytic reduction of nitrogen oxides (DeNOx-SCR) [1]. In this work, we investigated the design and improvement of zeolite-based catalysts for DeNOx-SCR reaction by combining experimental methods and density functional theory (DFT). Several catalysts were synthesized, and their activity and selectivity were screened under various operating conditions. After screening, the best performing catalysts were thoroughly characterized and modeled using DFT-based methods.

Identification of key reaction intermediates provided mechanistic insights for DFT modeling and enabled us to propose multiple, simultaneous reaction pathways. The findings deepen the understanding of zeolite-based DeNOx-SCR catalysts and provide guidelines for optimization and deliberate design.

References:

[1] Y. Xin, Q. Li, Z. Zhang, *ChemCatChem* **10** (2018) 29-41.