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Abstract

Toluene oxidation on metal-oxide catalysts: Theoretical modeling

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Abstract:

Removal of reactive organic species from the environment becomes a standard in modern society. In many reactions catalytic centers are used to enable reactions which would otherwise be energetically demanding. Apart from the activity of the catalyst, the material availability and the cost of production of the catalyst should also be taken into account. Here, several relatively inexpensive materials are investigated as potential catalysts for toluene degradation.

Interaction of toluene in oxygen atmosphere has been investigated by modeling the most abundant fraction in several powder catalysts as investigated in toluene degradation experiments. The repeated unit cell has been formed from MnO2, Mn2O3, Fe2O3, NiO and CuO crystal slab consisting of approximately 1000 atoms from crystal surrounded by vacuum layer to which three or four toluene and oxygen molecules were added. For calculation, the reactive force-field method was used as implemented in the ReaxFF code developed and by Duin et al [1]. Although a semiempirical method, this code has shown considerable success in modeling binding, due to the implemented bond order changes depending on the interatomic distances [2]. Temperature controlled Berendsen thermostat (NVT) with damping constant of 0.1 fs is used for 2.5fs molecular dynamics (MD) calculation on the initially energy minimized crystal structure at 500K. Toluene is then added and additional 25ns

MD calculation is performed (100000 steps of 0.25fs) at 500K. Additionally, calculations involving temperature rise from 500K to 700K, followed by 6.25 fs calculation at 700K and then temperature drop back to 500K were performed keeping all the other parameters as in constant temperature calculations. These were done in an attempt to model the much longer time available for reactions under experimental conditions more realistically. Unfortunately the experimental times of the order of 1s are not accessible to the MD model due to time and size limitations.

Biography:

Vjeran Gomzi has graduated at Faculty of Science in Zagreb in the field of Medical physics in 1999. In 2007 he obtined his PhD from the same Faculty in the field of Biophysics. He has been working as a PhD student at the Faculty of Pharmacy and Biochemistry and as the postdoc at the Rudjer Boskovic Institute in Zagreb. He is the author of 27 scientific papers in the fields of Computational Physics, Biophysics, and Theoretical chemistry. Since 2018 he holds the position of Assistant professor at the Applied Physics Department at Faculty of Electrical Engineering and Computing in Zagreb.

Publication of speakers:

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