Insight Medical Publishing

Archives in Chemical Research

ISSN 2572-4657

2020

Vol.4 No.5

Toluene oxidation on metal-oxide catalysts: Theoretical modeling

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Abstract

Removal of reactive organic species from the environment is often done using catalytic centers. Apart from the activity of the catalyst, the material availability and the cost of production of the catalyst are important. Here, several inexpensive materials are investigated as potential catalysts for toluene degradation.

Toluene adsorption on MnO_2, Mn_2O_3, Fe_2O_3, NiO and CuO was theoretically investigated. Unit cell has been formed from crystal slab of approximately 1000 atoms surrounded by vacuum layer to which toluene and oxygen molecules were added. The reactive force-field (ReaxFF) method was used. Temperature controlled Berendsen thermostat (NVT) is applied for 2.5fs molecular dynamics (MD) calculation on energy minimized crystal structure. Toluene is added and additional 25ns MD calculation is performed at 500K. Calculations involving temperature rise from 500K to 700K, followed by 6.25fs calculation at 700K and temperature drop back to 500K were performed to model much longer time available under experimental conditions.

The catalyst potential for toluene adsorption and catalytic activity is evaluated by the amount of free toluene molecules as function of time. It is found that the structures investigated showed behavior which is related to the O_2 and toluene binding energies. The largest catalytic activity is observed for Fe_2O_3 and MnO_2, while CuO did not show any toluene adsorption or degradation. While Fe_2O_3 activity seems to be the result of large toluene adsorption energy, MnO_2 structure additionally offers crystal surface oxygen and show the contribution to the activity from surface dynamics and structure (including oxygen diffusion, defects, etc.).

Biography:

Vjeran Gomzi has graduated at Faculty of Science in Zagreb in the field of Medical physics. In 2007 he obtained his PhD from the same Faculty in the field of Biophysics. He is the author of 27scientific papers in the fields of Computational Physics, Biophysics, and Theoretical chemistry. Since 2018 he holds the position of Assistant professor at the Faculty of Electrical Engineering and Computing in Zagreb.

Speaker Publications:

1. "Metal Cluster (M-2-M-60, M = Au, Cu, Ni, Pt) Formation as Investigated Using the Reactive Force Field" Journal of Computational and Theoretical Nanoscience/ 2012/ 9(3):419-427.
2. "Fluxionality of hydrogen ligands in Fe(H)2(H2)(PEtPh2)3" Inorganic Chemistry/ 2011/ 50(21):10740-7
3. "Modeling of the bis(glycinato)copper(II) cis-trans isomerization process: Theoretical analysis" Journal of Structural Chemistry/ 2011/ 52(5)
4. "DFT study of radicals formed in 2-thiothymine single crystals at 77 K: 1- and 2-molecule models revised" Computational and Theoretical Chemistry/ 2011/ 963(2):497-502
5. "Structure Prediction of Bis(amino acidato)copper(II) Complexes with a New Force Field for Molecular Modeling" Journal of Chemical Theory and Computation/ 2009/ 5(7)

7th World Congress on Chemical Engineering and Catalysis Webinar– July 22-23, 2020.

Abstract Citation:

Vjeran Gomzi, Toluene oxidation on metal-oxide catalysts: Theoretical modeling; Chemical Engineering Congress2020, 7th World Congress on Chemical Engineering and Catalysis-Webinar July22-23, 2020.

(https://chemicalengineering.annualcongress.com/abstract/2020/toluene-oxidation-on-metal-oxide-catalysts-theoretical-modeling)