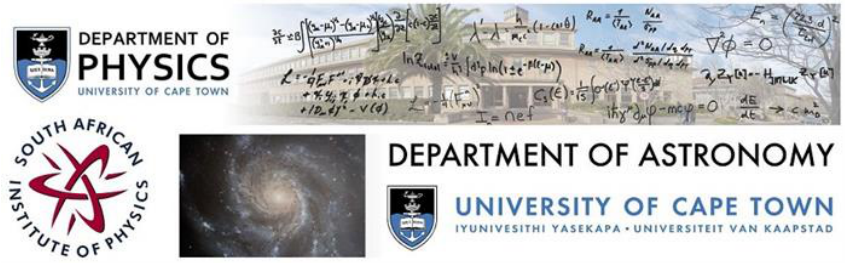

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The SCC-DFTB study of H₂O interaction with TiO₂ supported Pd catalyst

Tuesday, 5 July 2016 15:20 (20 minutes)

Abstract content
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The supported metal nanoparticles are of great importance in many industrial catalytic processes, such as oxidation of methane, carbon monoxide and formic acid. In particular, the platinum group metals (PGM) such as Pd, Pt and Rh supported on metal oxides are being considered. Palladium is often used as a catalyst for many processes in emissions control technologies. This is due to its potential of becoming a novel catalyst for low temperature methane combustion.
During the methane oxidation, H₂O is produced and it is important to understand the behaviour of this molecule as it gets in contact with catalyst. The interaction of H₂O molecules with Pd nanoclusters and TiO₂ supported Pd nanoclusters were investigated using the self-consistent-charge density functional tight binding (SCC-DFTB) approach as implemented within the DFTB+ code [5]. Firstly, the interaction of H₂O molecule with Pd₁₃ nanocluster was investigated. The results show that when H₂O interact with Pd nanoclusters, it dissociate into OH and H forming a Pd − O bond length of 1.992 Å and Pd − H bond length of 1.571 Å, respectively. Secondly, the interaction H₂O with TiO₂(101) supported Pd₁₃ on various adsorption sites preferred the bridge adsorption site, however no dissociation was observed. This gave an average bond length of 1.979 Å with adsorption energy of -1.887 eV.
Lastly, molecular dynamics (MD) calculations were performed on the most preferred orientation of H₂O adsorbed on TiO₂(101) supported Pd₁₃ system. It was obtained that the H₂O molecule dissociates into OH and H at about 598 K.

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PE Ngoepe
Phuti.Ngoepe@ul.ac.za
University of Limpopo

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Primary author: Ms CHUMA, Moyahabo Hellen (University of Limpopo)

Presenter: Ms CHUMA, Moyahabo Hellen (University of Limpopo)

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