



Contribution ID: 397

Type: Oral Presentation

The SCC-DFTB study of H_2O interaction with TiO_2 supported Pd catalyst

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

Abstract content (Max 300 words) http://events.saip.org.za/getFile.py?target=_blank Formatting & Special chars

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, H_2O is produced and it is important to understand the behaviour of this molecule as it gets in contact with catalyst. The interaction of H_2O molecules with Pd nanoclusters and TiO_2 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 H_2O molecule with Pd_{13} nanocluster was investigated. The results show that when H_2O 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 H_2O with $\text{TiO}_2(101)$ supported Pd_{13} 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 H_2O adsorbed on $\text{TiO}_2(101)$ supported Pd_{13} system. It was obtained that the H_2O molecule dissociates into OH and H at about 598 K.

Apply to be considered for a student award (Yes / No)?

yes

Level for award (Hons, MSc, PhD, N/A)?

PhD

Main supervisor (name and email) and his / her institution

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

**Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?**

No

**Please indicate whether
this abstract may be
published online
(Yes / No)**

No

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

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

Session Classification: Division for Physics of Condensed Matter and Materials (1)

Track Classification: Track A - Division for Physics of Condensed Matter and Materials