Contribution ID: **271** Type: **Poster Presentation**

First principles studies of Palladium nanoparticles on TiO₂ surfaces for catalytic application

Tuesday, 26 June 2018 15:00 (2 hours)

Palladium-based catalyst are being developed as an alternative to the commonly used and high cost platinum catalyst because of their similar electronic configurations, lattice constants and they are cheaper than platinum with a high methanol-tolerance. In this study, first principle density functional theory was used to study the catalytic properties of Pd/TiO₂, in particular the interaction and electronic behaviour of palladium nano-clusters on a stable titanium dioxide surface using the plane-wave pseudo-potential method. Titanium dioxide is used as a metal support to develop the palladium catalyst, and is the most important transition metal oxide since its photo-catalytic activity was discovered. This transition metal oxide was used in many catalytic processes in the industries such as metal catalysts, which include the platinum group metals such as Pd, Pt, and Rh. These metals are involved in processes such as fuel cells, methane oxidation, catalysis, and in emission control technology. Firstly, the stability of titanium dioxide polymorphs was deduced from elastic properties and in good agreement with the experimental values to within 3%. The observation made was based on the shear modulus of rutile being higher and positive compared to that of the other polymorphs suggesting that rutile is more stable. The order of surface stabilities is given as (110)> (100)> (101)> (001)> (111), and in good agreement with previous work. Adsorption of water on the stable (110) surface showed that the (110) surface was more preferred(exothermic). Secondly, the interaction of Palladium clusters with titanium dioxide surface showed that Pd₁₃ prefers the bridging adsorption site, and as predicted it's the least negative D₂E energy value. The findings of this work suggests that palladium-based catalysts may play a significant role in future developments and applications in emission control technologies.

Please confirm that you
have carefully read the
abstract submission instructions
under the menu item
"Call for Abstracts"
(Yes / No)

Yes

Consideration for
student awards
Choose one option
from those below.
N/A
Hons
MSc
PhD

Hons

Supervisor details
If not a student, type N/A.
Student abstract submision
requires supervisor permission:
please give their name,
institution and email address.

Prof Hasani Chauke, University of Limpopo hasani.chauke@ul.ac.za
Prof Phuti Ngoepe , University of Limpopo phuti.ngoepe@ul.ac.za

Primary authors: Ms MAZIBUKO, Andile (yes); Prof. CHAUKE, Hasani (University of Limpopo); Prof. NGOEPE, Phuti (University of Limpopo); Ms DIALE, Refiloe (University of Limpopo)

Presenter: Ms MAZIBUKO, Andile (yes)

Session Classification: Poster Session 1

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