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## **First principles studies of Palladium nanoparticles on TiO<sub>2</sub> surfaces for catalytic application**

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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/TiO<sub>2</sub>, 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 Pd<sub>13</sub> prefers the bridging adsorption site, and as predicted it's the least negative D<sub>2</sub>E 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.

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