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Computational modelling studies of O2/Pt surface for fuel-cell application

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Ab-initio density functional theory with the generalized gradient approximation was used to investigate the interaction of oxygen molecule with the Pt (100), (110) and (111) surfaces. The oxidation of Pt may lead in the development and enhancement of the catalytic activity of fuel-cells, especially those operating at low temperatures, such as proton exchange membrane fuel cells and proton conducting membrane fuel cells. The optimization of the non-adsorbed platinum surfaces reflected that the (111) surface is the most stable surface. Three adsorption sites were considered, the bridge, hallow and Pt-top. For oxygen molecule adsorption on Pt, we observed a superoxide (Pt-O-O) formation on (100) surface while on (110) surface a bridge bonding (Pt-O-O-Pt) is observed. The adsorption energy indicated that on the (100) surface, the Pt-top adsorption site is more exothermic than bridge and hollow sites. Furthermore, the electronic density of state show strong Pt 3d and O 2p hybridization which is attributed to the strong adsorption energy.

Apply to be
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No

Level for award
 (Hons, MSc,
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N/A

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

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Would you like to
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Yes

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