



SDI Review Form 1.6

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| Journal Name: | International Research Journal of Pure and Applied Chemistry |
| Manuscript Number: | Ms_IRJPAC_27627 |
| Title of the Manuscript: | MODELING ELECTROCATALYTIC ACTIVITY OF NITROGEN RADICALS |
| Type of the Article | |

General guideline for Peer Review process:

This journal's peer review policy states that **NO** manuscript should be rejected only on the basis of '**lack of Novelty**', provided the manuscript is scientifically robust and technically sound.

To know the complete guideline for Peer Review process, reviewers are requested to visit this link:

(<http://www.sciencedomain.org/page.php?id=sdi-general-editorial-policy#Peer-Review-Guideline>)



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PART 1: Review Comments

| | Reviewer's comment | Author's comment <i>(if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)</i> |
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| <u>Compulsory</u> REVISION comments | None | |
| <u>Minor</u> REVISION comments | <ol style="list-style-type: none"> 1. In line 71, 72 and 75, the author said "The structures have no imaginary frequencies." How do the author get this information? The authors should provide the evidences. 2. All the figures should be re-plotted to show the structure more clearly. 3. H₂O instead of O₂H may be better. | <p>Imaginary frequencies are indicated in the output of Gaussian by minus signs. I have put a sentence into the manuscript explaining this. The figure have been re-drawn using Chem Draw 2D Pro software.</p> <p>O₂H has been changed to HO₂</p> |
| <u>Optional/General</u> comments | The author study the role of nitrogen radicals in the reactions at the cathode of fuel cells using DFT method, and find that O ₂ and H O ₂ can adsorb on nitrogen radicals and can be a catalyst for the reactions at the cathode. This is very interesting and meaningful for the application of nitrogen radicals in fuel cells. | |