



**SDI Review Form 1.6**

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| Journal Name:            | <a href="#">International Research Journal of Pure and Applied Chemistry</a> |
| Manuscript Number:       | <b>Ms_IRJPAC_27627</b>   |
| Title of the Manuscript: | <b>MODELING ELECTROCATALYTIC ACTIVITY OF NITROGEN RADICALS</b>               |
| 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**

|  | <b>Reviewer's comment</b>   | <b>Author's comment</b> <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> |
|--|---|---|
| <b><u>Compulsory</u></b> REVISION comments | No  |   |
| <b><u>Minor</u></b> REVISION comments      | <p>1. I think the English in article needs polishing. For example, page 2 line 50 "the minimum energy structures" should be replaced by "structures of the minimum energy".</p> <p>2. The atomic structure (Fig. 1-6) is more satisfying if the authors could redraw them with the professional software.</p> | <p>I have gone through the manuscript and tried to improve the English</p> <p>The figures have been redrawn using Chem 3D pro software.</p>   |
| <b><u>Optional/General</u></b> comments    | <p>1. The authors only calculated the BDE to explain the effect of the nitrogen radicals. The result is inadequate to support their conclusion. I think it needs to add other results (i. e.: the electronic structure of the atomic model) and further discussion.</p>                                       | <p>Adsorption energies were also calculated not just BDEs</p>   |