



SDI Review Form 1.6

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 (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)
<u>Compulsory</u> REVISION comments		
<u>Minor</u> REVISION comments	<p>1. Is there any effect of the supports (e.g., carbon nanotube paper) on the catalytic activities of the nitrogen radicals? Is it possible to examine those effects by DFT, if any?</p> <p>2. Grammatical check and correction are needed. Also, the level of artwork should be improved.</p>	<p>The CNT paper does not contribute to the catalytic effect. Measurements made on the carbon nanotube paper without the nitrogen radicals showed no catalytic effect.</p> <p>The figures have been redrawn using Chem Pro 3D software..</p> <p>The manuscript has been reviewed and corrected for grammatical errors.</p>
<u>Optional/General</u> comments	<p>This work uses DFT to describe the adsorption of O₂ and O₂H on nitrogen radicals and the subsequent catalytic dissociation reactions that produce O and OH species participating in the reactions at the cathodes of fuel cells. The results suggest that N₈⁻ and N₄⁻ radicals have catalytic effects on the O₂H dissociation reaction, being consistent with experimental observation and meaningful in prediction of new catalysts.</p>	