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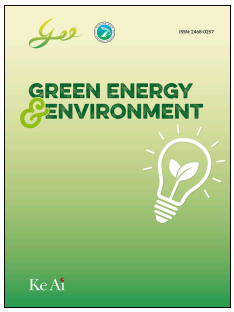

Insights into Electrochemical CO_2 Reduction on Tin Oxides from First-principles Calculations

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To: *Green Energy & Environment (GEE)* Editor
Subject: Manuscript for SI **New Energy Catalysis**

Title: **Insights into Electrochemical CO_2 Reduction on Tin Oxides from First-principles Calculations**
Subject: Surfaces, Catalysis, CO_2 reduction
Author: Siwen Wang (PhD student), Jiamin Wang (PhD student), and Hongliang Xin (Assistant Professor)

Dear Prof. Zhang:

Thank you for the invitation for this special issue focusing on New Energy Catalysis. We are excited to present our recent work on CO_2 electroreduction on Sn-based catalysts which has potential in both energy storage and alleviating CO_2 problem, fitting well to this theme. Herein we are employing quantum chemical calculations for understanding complex mechanisms of CO2 electroreduction on SnO model surfaces for producing formic acid and CO. By developing models that pinpoint the stable surface structures under relevant conditions and describe the general trend of selectivity, we are proposing the reactivity descriptor, i.e., the *CO2 free formation energy, that can be used for guiding the design of improved catalysts, such as by strain engineering.

The proposed model presented in the paper will be critical for understanding catalytic CO2 reduction mechanisms and developing improved catalysts, and as such we believe that it is of great interest to the broad readership of your journal. The study opens a new way for designing strained metal oxides catalysts with improved performance.

We assure that the manuscript is not under consideration for publication and has not been published elsewhere.

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