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The Role of Metal-Oxo Intermediate to Oxygen Reduction Reaction Catalysis: A Theoretical Investigation Using Nitrogen-Substituted Carbon Nanotube Models

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Highlights

- Qualitative characterizations for the metal-based oxygen reduction reaction (ORR) mechanism for the common transition metal catalyst by Density Functional Theory.
- Identifying the important role of oxo-metal intermediate for providing the uniform stepwise free energy and the generation of electric potential of ORR.
- Differentiating 2e vs. 4e pathway of ORR mechanism between group 8 and 9 metal centers in the implication of electric current generation via *OOH bond breaking barrier.

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