Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Insights into the origin of Co-based bimetallic catalysts with para-structure exhibiting ORR and OER bifunctional activity

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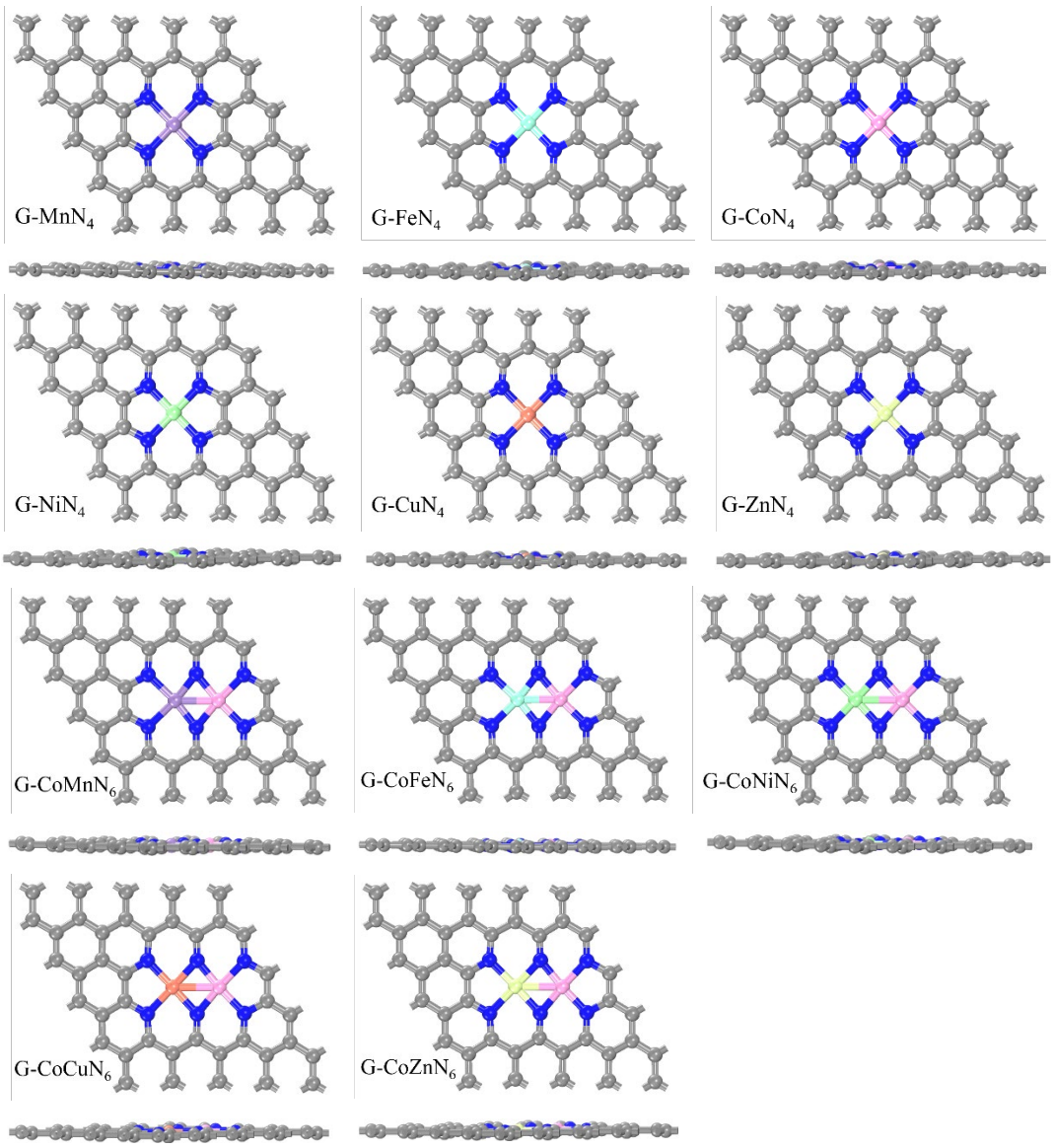
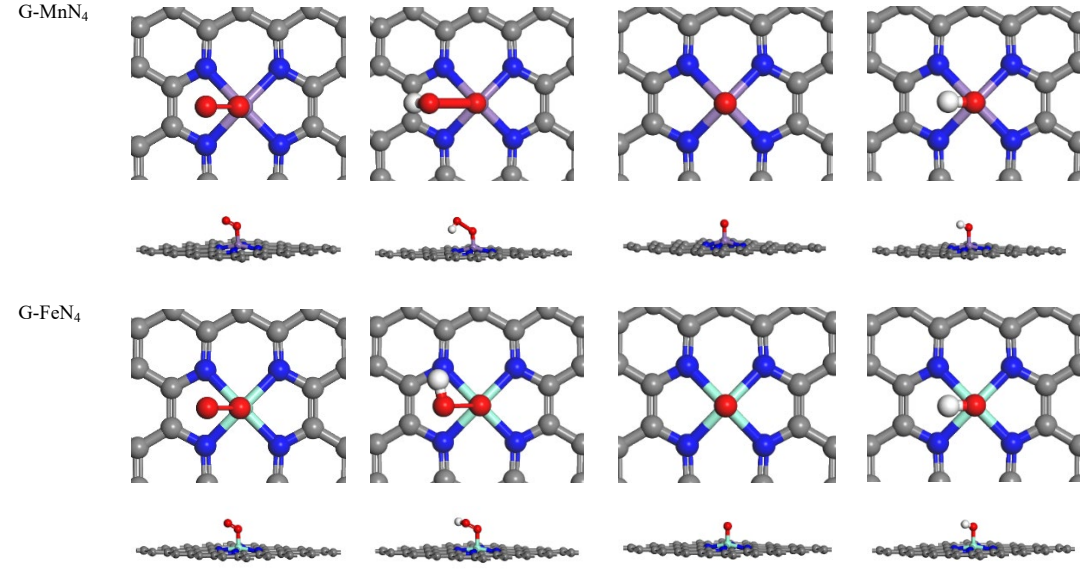
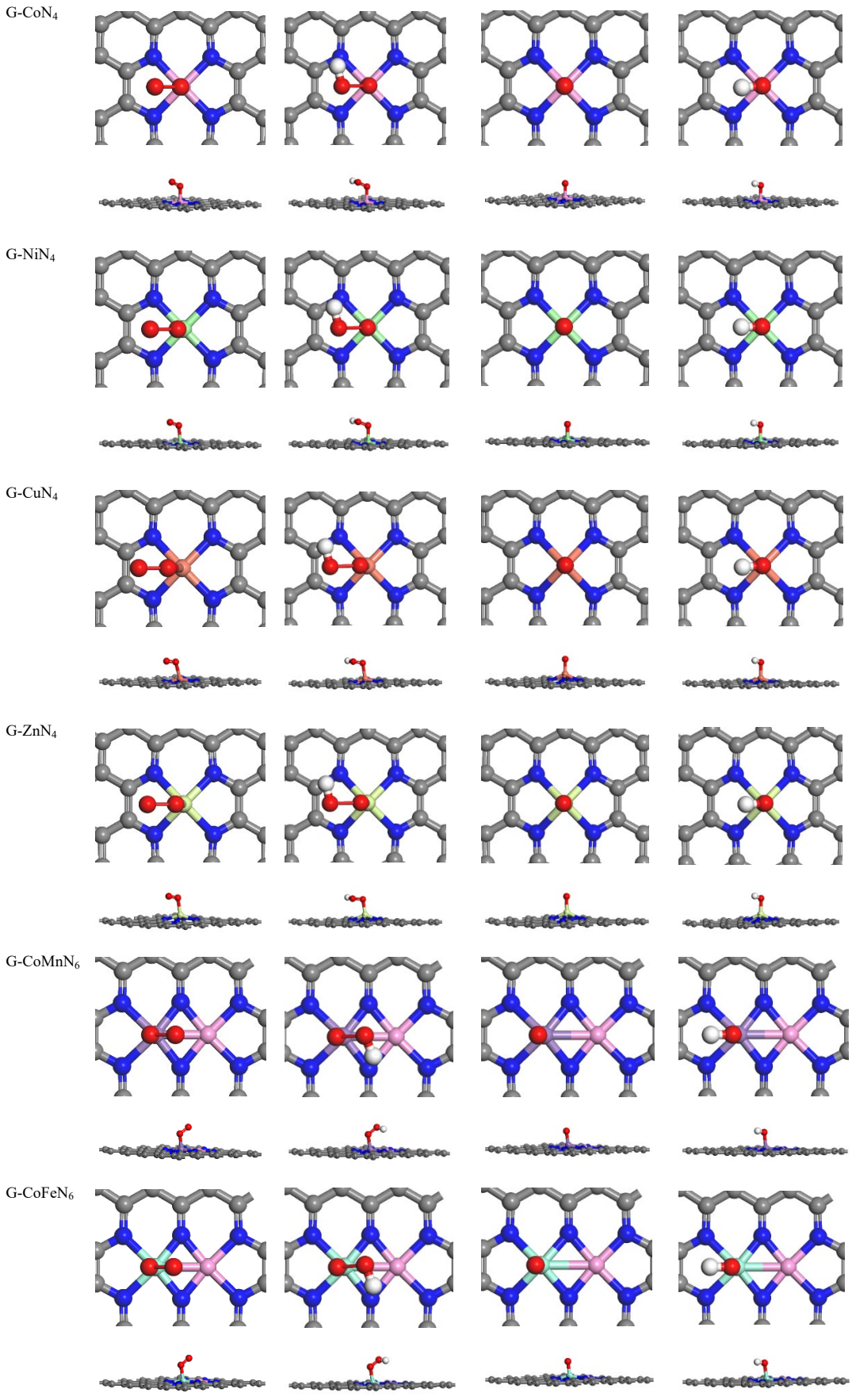


Fig. S1. The structures of single metal atom catalysts and bimetallic catalyst after optimization.




G-CoN4
G-NiN4
G-CuN4
G-ZnN4
G-CoMnN6
G-CoFeN6

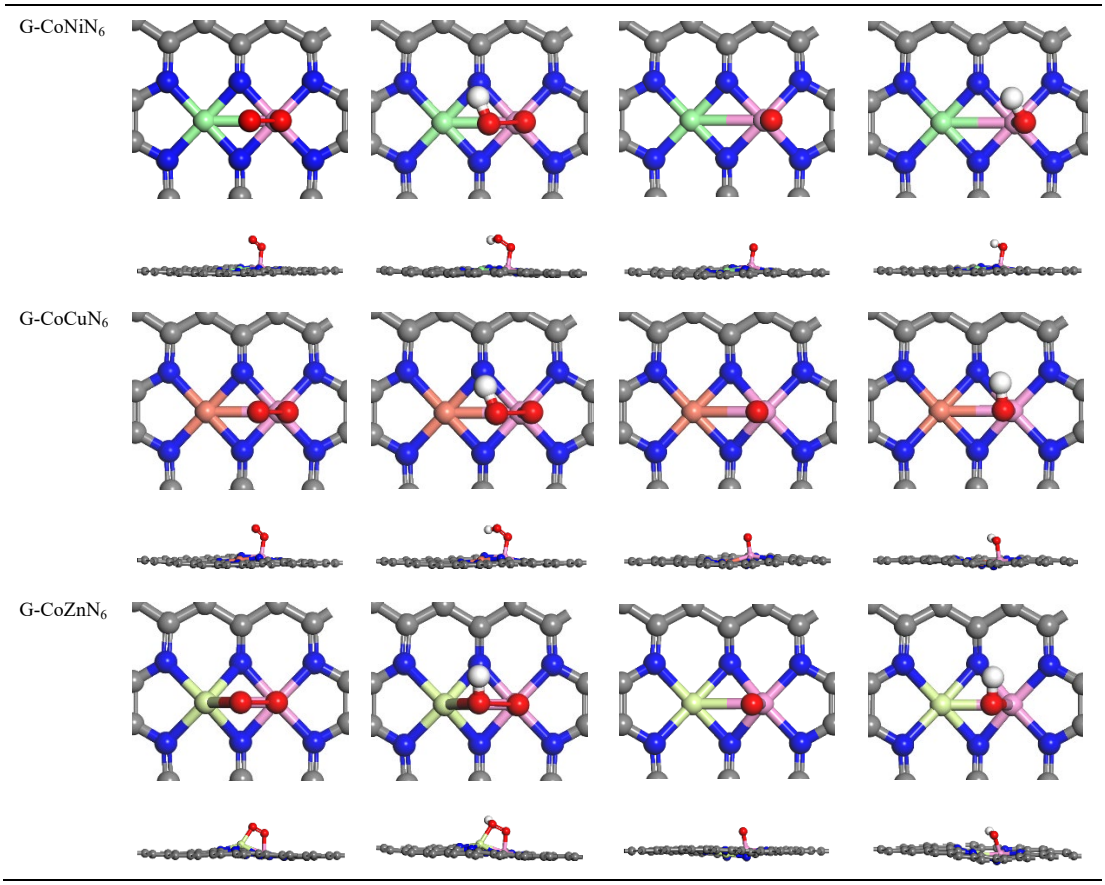


Fig. S2. Adsorption configurations of various oxygen-containing species on single metal atom catalysts and Co-based bimetallic catalysts.

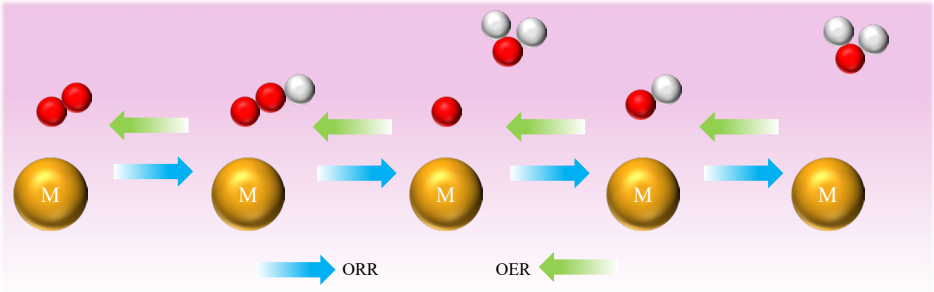


Fig. S3. Four-electron reaction of ORR and OER in acidic media.