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Rational Design of Two-Dimensional Organic Frameworks for Energy Conversion

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Two-dimensional (2D) metal-loaded organic frameworks (MOFs) have a high specific surface area, adjustable structural composition and uniform surface active sites, making them ideal catalysts for energy conversion. However, the large pore structure limits the effective transmission of electrons. Designing 2D MOFs with high stability and high conductivity is the key to obtaining an efficient electrocatalyst.[1] By performing first principles calculations, we designed a series of 2D MOFs by coupling conjugated organic ligands with four-coordinated transition metals, and applied them to various electrocheimcal reactions, including oxygen reduction reaction, oxygen evolution reaction, nitrogen reduction reaction and carbon dioxide reduction reaction.[2,3] The computational results show that variation of metals and coordination environments can not only allow the formation of stable d-π conjugated structures, but also enable the adjustment of catalytic activity. The designed 2D MOFs with Co centers exhibit higher electrocatalytic activity than traditional precious metal catalysts. With the help of the state-of-the-art methods, we revealed the relationship between lattice, composition and catalytic activity,[4] providing rationale for the design of effective catalysts for energy conversion.

References

[1] Y. Jing et al, *Trends Chem.* **2022**, *4*, 792.
[2] T. Liu et al. *J. Phys. Chem. Lett.* **2024**, *15*, 6216.
[3] L. Hu et al, *J. Phys. Chem. Lett.* **2023**, *14*, 11429.
[4] T. Li et al. *ACS Catal.* **2024**, *14*, 7220.