



Showcasing research from Professor Yirong Mo's laboratory, Joint School of Nanoscience and Nanoengineering (JSNN), University of North Carolina at Greensboro (UNCG), NC, USA.

Toward tuning the bandgap in *meta*-substituted Fe-MOFs

We examine the bandgap, HOMO, and LUMO energy level trends in MOF-5 fully transmetalated with iron (*i.e.*, Fe-MOF-5), as a function of the substituent effect (in the term of Hammett constant σ_m) and solvent effect (in the term of dielectric constant ϵ). Computational results along with the polynomial equations of fit from statistical analysis suggest that the bandgap in these transmetalated models is significantly influenced by the dipole-induced dipole interactions. These results provide insight into the impact of shifting interactions of σ_m and ϵ on the bandgap of Fe-MOF-5.

As featured in:



See Daniel J. C. Herr,
Yirong Mo *et al.*,
Mater. Adv., 2024, 5, 6842.