2D conductive MOF electronic property study

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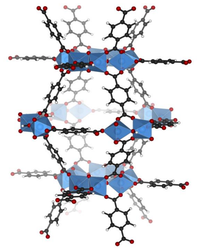
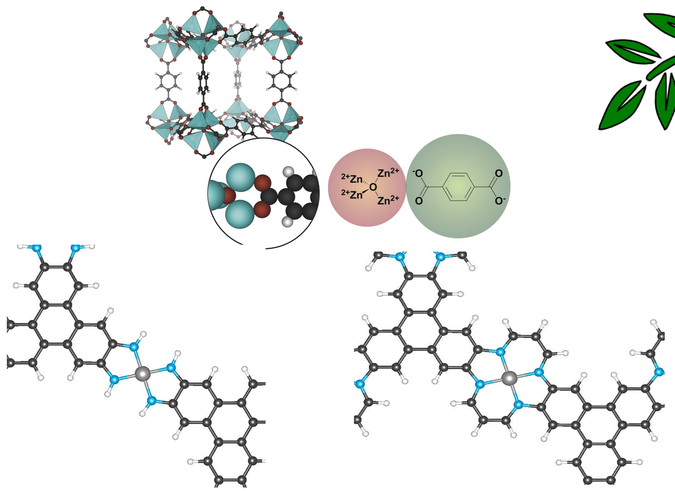
Hendon Materials Simulation

Metal Organic Framework

Gas storage
Electro-catalysis
Energy storage
Sensors
Electronic devices



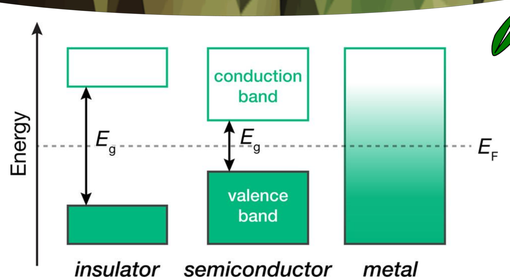
Charge localization problem:
Ionic interaction prevent charge delocalization between the metal cluster and the organic linker →large band gap →Terrible conductor



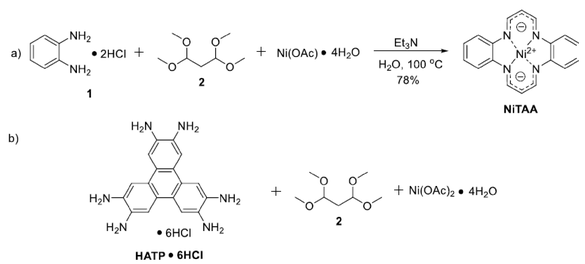
Conductivity: 40 S/cm

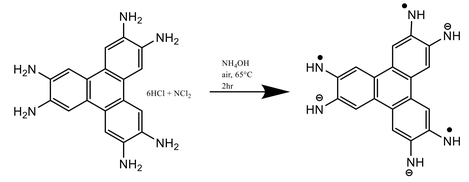
Conductivity: 10^{-10} S/cm

Band Structure



Linker formation





Results

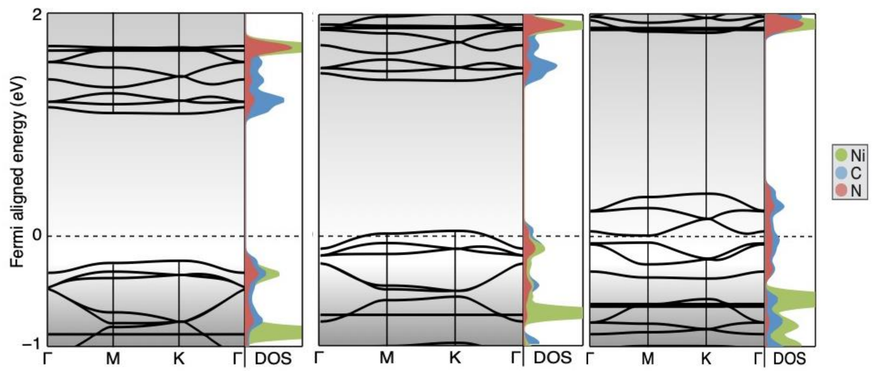


Figure 1. NiTAA-MOF monolayer band structure. (left) Neutral charge monolayer (middle) +1 charge monolayer (left) +6 charge monolayer

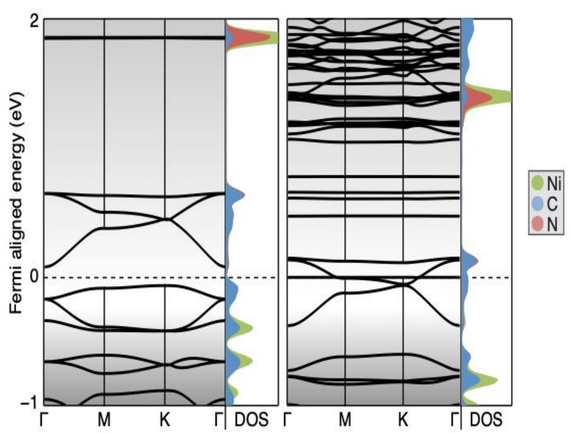


Figure 2. $Ni_3(HITP)_2$ monolayer band structure. (left) Neutral charge monolayer (right) -6 charge monolayer

Conclusion

Base on computational band structure result, Neutral charge NITAA-MOF is an insulator, while +1 and +6 showing matalic feature and semi-conductor feature, respectively. While HITP linker truncate oxidation state both remain unoxidized between NiTAA-MOF^{+6} and $Ni_3(HITP)_2^{-6}$, NiTAA-MOF^{+6} show semi-conductor behavior while $Ni_3(HITP)_2^{-6}$ shows metallic behavior. Bulk material and effect of metal exclusion still need to be further studied.

Materials and methods

All calculations were performed within the Kohn-sham DFT framework as implemented in Vienna ab intitio simulation package (VASP). Optimization calculation of NiTAA and $Ni_3(HITP)_2$ monolayer was both optimized under ionic relaxation of NSW=100 and ISIF=2. KPOINTs=auto while bulk material was done under ISIF=3.Electron density map was obtained through LPARD=TRUE base on optimized geometry of each model.

Band structure calculation were done under PBEsol exchange-correlation functional with Grimes dispersion (IVDM=12) factor included.

Reference

J. Am. Chem. Soc. 2019, 141, 42, 16884–16893

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Chem. Rev. 2020, 120, 16, 8536–8580

Acknowledgments

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