Meyer

U.S. DEPARTMENT OF ENERGY | Office of Science

Optimizing Excitation Energy Flow in Metal-Organic Framework Materials

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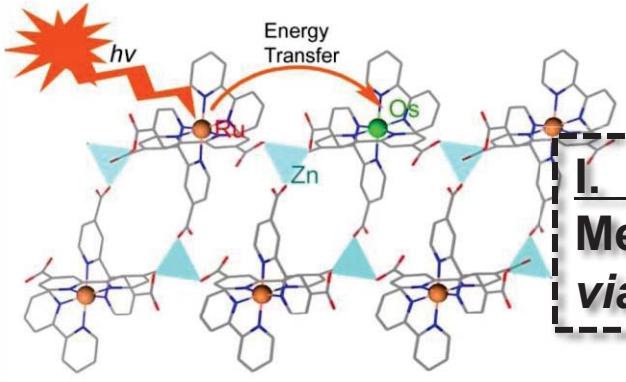
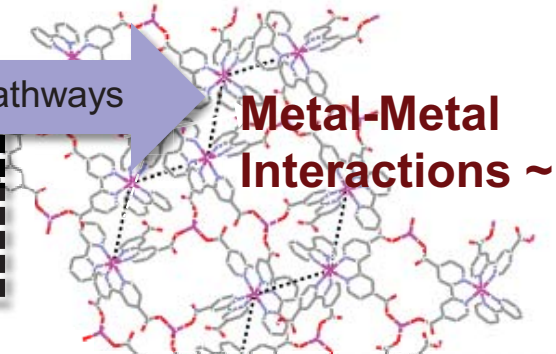


Kent, C.A.; Mehl, B.P.; Ma, L.; Papanikolas, J.M.; Meyer, T.J.; Lin, W. *J. Am. Chem. Soc.* **2010**, *132*, 12767.

I. Calculate:
Metal-metal couplings *via* atomistic models

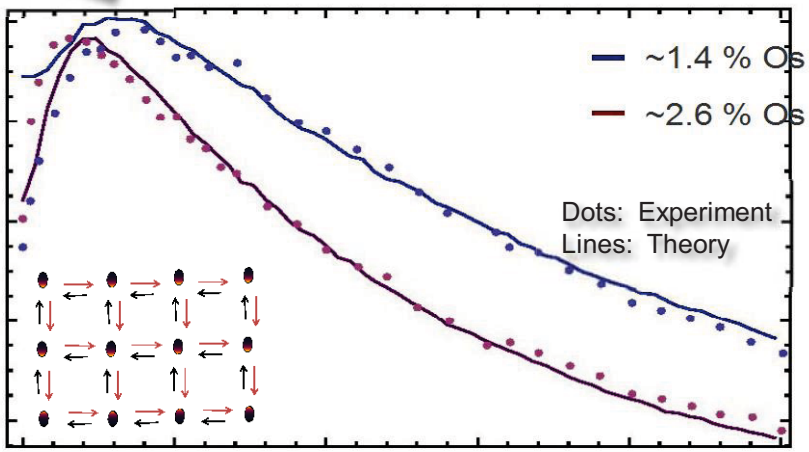
Find 1D Pathways



Metal-Metal Interactions ~ 10^{-4} eV

Reproduce Kinetics

II. Simulate:
Time-resolved emission with lattice master equations



Significance:

- Doped *metal-organic framework materials* (MOFs) are **promising for solar-energy collection and concentration**.

Achievements:

- Discovered **1D energy flow pathways** in Ru-Os MOFs;
- Lattice **kinetic models describe experimental time-resolved emission** @ Os doping levels;
- Now **optimizing MOF structures for excitation energy efficiency and energy delivery**.

SOLAR FUELS & NEXT GENERATION PHOTOVOLTAICS

UNC College of Arts & Sciences | Duke University | North Carolina Central University | NC State University | RTI International | UF University of Florida