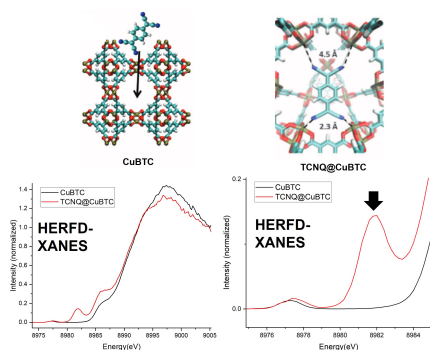


## PROBING HOST-GUEST INTERACTIONS IN CONDUCTIVE COPPER-BASED METAL ORGANIC FRAMEWORKS USING HIGH-RESOLUTION X-RAY ABSORPTION SPECTROSCOPY

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Metal-organic framework (MOF) materials are porous coordination polymers that have gained interest due to the tunability of the guest and host structures. This tunability can be particularly useful in electroconductivity applications yet has been challenging to implement due to their intrinsic insulating nature. Exploring ways to tune the electronic structure to promote electron migration is a key component in furthering research for applications that rely on conductivity such as electrocatalysis and sensing. Introduction of redox active guest species into effectively insulating MOF structures is one strategy being explored to impart electrical conductivity. This talk will focus on one particular host-guest system: a  $\text{Cu}_3(\text{BTC})_2$  MOF (; BTC=benzene 1,3,5-tricarboxylic acid) infiltrated with redox active 7,7,8,8-tetracyanoquinodimethane (TCNQ) guest molecules. It has been reported previously that the introduction of TCNQ into the pores  $\text{Cu}_3(\text{BTC})_2$  leads to an increase in conductivity. A key component of un-

derstanding this system is the interaction occurring between the copper sites of the framework and TCNQ guest molecules. A fundamental study using vibrational and X-ray spectroscopy were used to further understand this interaction. Copper K-alpha, resonant X-ray emission spectroscopy (RXES) was used to specifically probe the Cu interaction with this redox active guest. HERFD XANES spectra extracted from the 2D RXES planes reveal subtle changes of the pre-edge features and additional edge features corresponding the pi-backbonding of the TCNQ cyano groups to the Cu sites in the framework. Cu K-edge data are supplemented by TD-DFT calculations to determine the orbital contributions to different edge features and therefore the nature of this host-guest interaction on a molecular level.