COPPER-PYRIDIL NANOPOROUS NETWORK ANALYSIS

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ABSTRACT

This study offers an in-depth spectroscopy and Scanning Tunneling Microscopy (STM) analysis of 1,3,5-tris[4-(pyridine-4-yl)phenyl]benzene (TPyPB) which on a Cu(111) surface formed a 2D molecular overlayers which at 400-500 K a honeycomb nanostructure emerges. Utilizing density functional theory (DFT) mainly with a Linear Combination of Atomic Combination of Atomic Orbitals (LCAO) and Real Space (RS) approach, we examined FTIR, Raman spectra, Density of States (DOS), Partial Density of States (PDOS), Optical Absorption Spectrum (OAS), and STM. These multiple analyses comprehensively understand the material's properties and behavior and provide future research insight and development of this material.

INTRODUCTION

Metal-organic frameworks (MOFs) and their unique properties show wide-ranging applications from catalysis and gas storage to photovoltaics and drug delivery[1] . However, the comprehensive theoretical analysis might show properties like photoelectric energy conversion[2]. This work underscores the characterzation of this nanoporous, providing the foundation for further studies and potential applications.

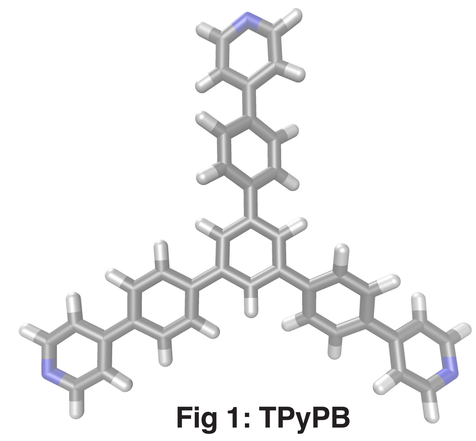


Fig 1: TPyPB

DFT

The relaxed TPyPB with Py-Cu-Py bonding mode on the Cu(111) surface is similar to ref.[3] in Fig (2.b). The TPyPB exhibited a twist due to their electronic density interaction. The Cu-N bonding mode presented 1.975 Å length.

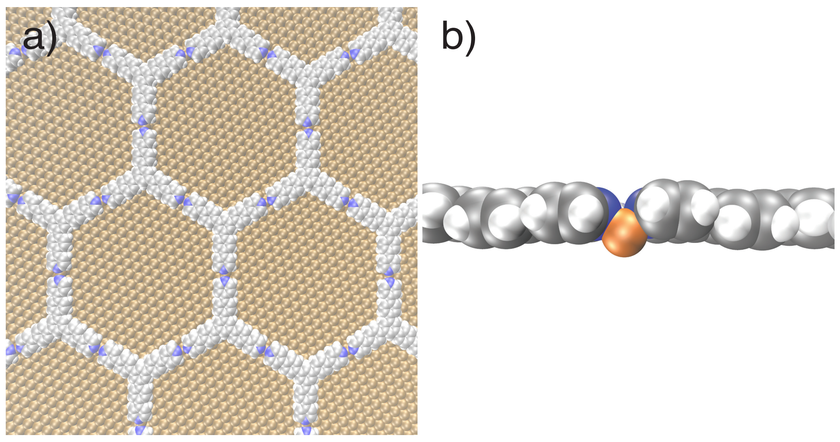


Fig 2: a) Nanoporous Network, b) N-Cu bonding mode

FT-IR

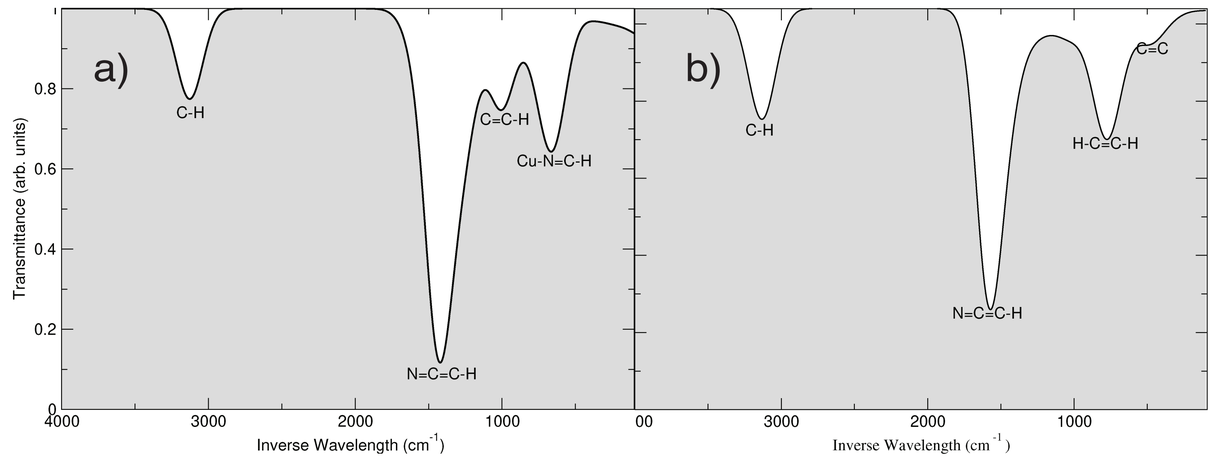


Fig 3: a) FT-IR Spectrum from TPyPB on Cu(111), b) FT-IR Spectrum from TPyPB on Isolated in Gas Phase.

PDOS

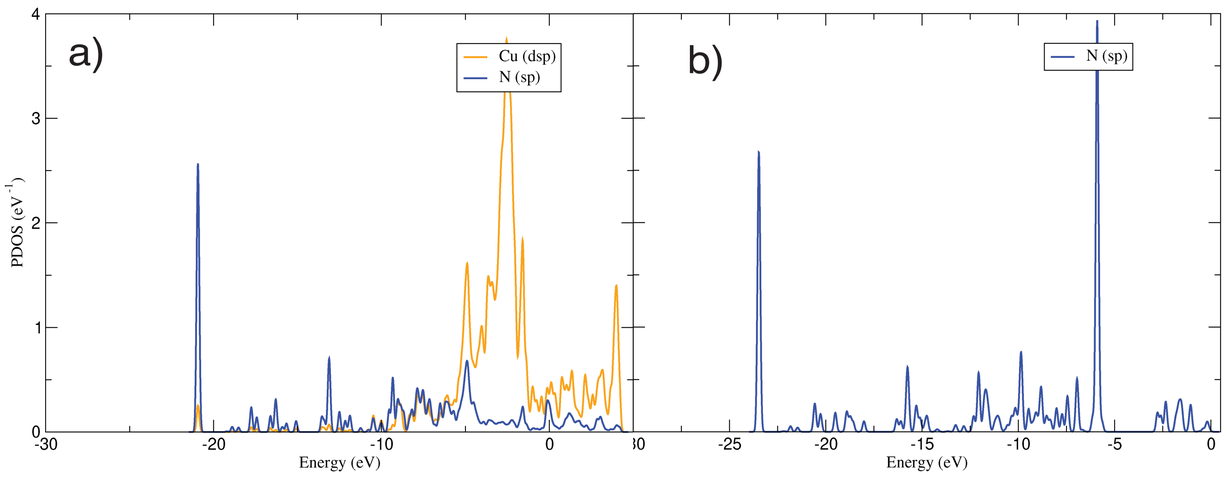


Figure 6: a) PDOS of Cu, and N of TPyPB on Cu(111) surface. b) PDOS of N atoms for Isolated TPyPB in Gas Phase. b) OAS for Isolated TPyPB

OAS

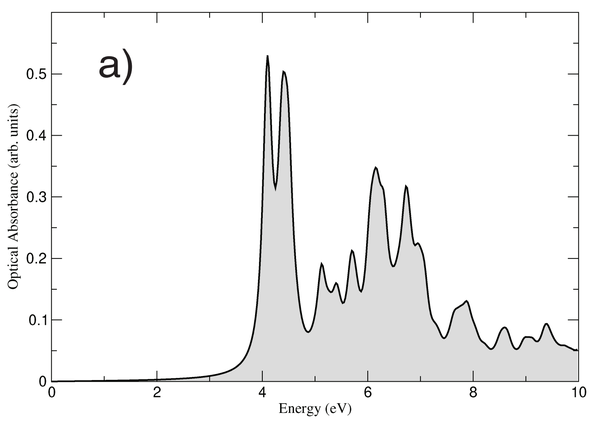


Fig 4: a) OAS for Isolated TPyPB b) OAS for Isolated TPyPB

RAMAN

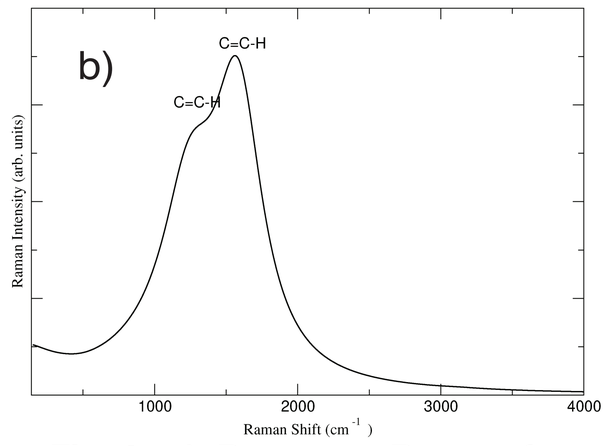


Fig 4: a) Resonant Raman for Isolated TPyPB in Gas Phase b) OAS for Isolated TPyPB

STM IMAGES 400 - 500 K

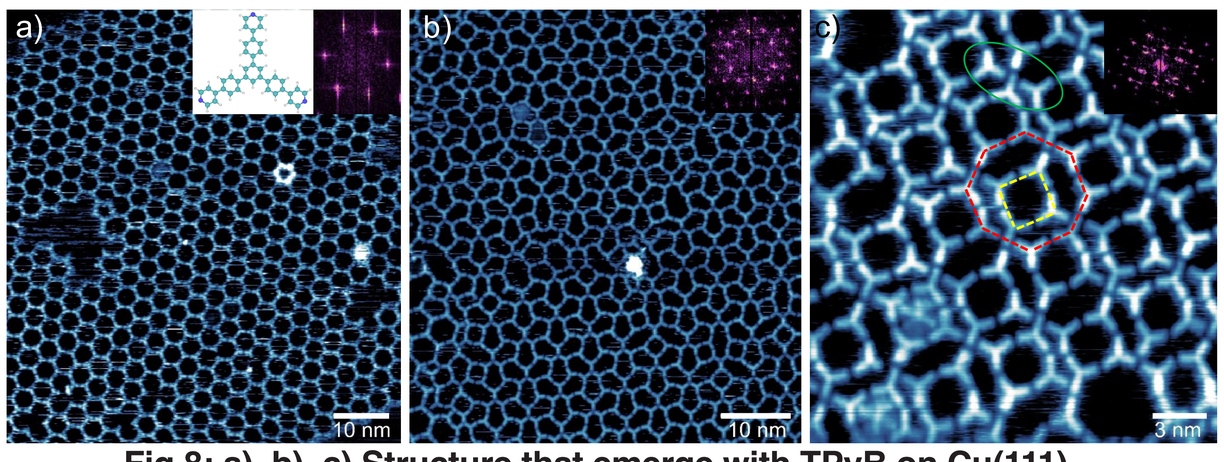
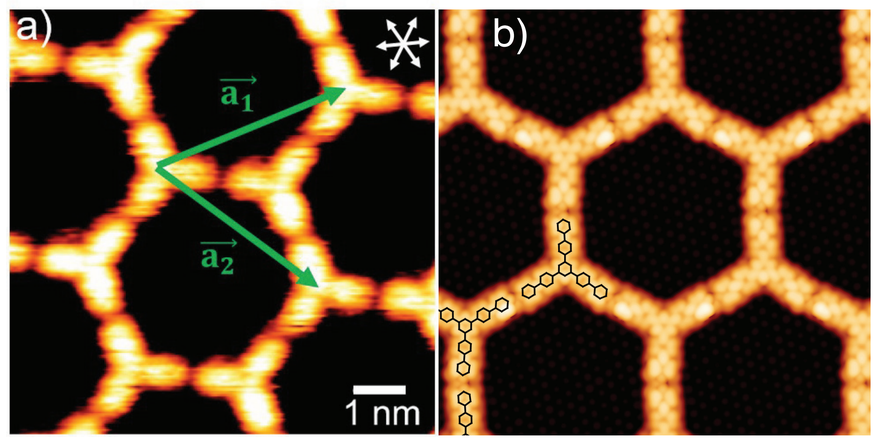


Fig 8: a), b), c) Structure that emerge with TPyB on Cu(111)

STM

Fig 8: a) High-resolution STM image of the honeycomb of the TPyPB network with the lattice vectors (Vbias = -1.4 eV) as Ref [4] b) STM simulations (Vbias = -0.41 eV at HOMO)



Computational Details

The calculations were made with PBE[5] and D3[6] with projector-augmented wave method (PAW[7] in GPAW), The STM image approximated with Tersoff-Hamann[8] in ASE[9].

$$I \propto \int_{\varepsilon_F}^{\varepsilon_F + eV} \sum_{kn} w_k \, |\Psi_{kn}(\mathbf{r})|^2 \, \delta(\varepsilon - \varepsilon_{kn}) d\varepsilon$$

Experimental Details

Performed in UHV at 10^{-10} mbar consist in two chambers the first equipped with X-ray photoelectron spectroscopy, LEED optics, Knudsen cell for molecular sublimation, e-beam evaporator for metal deposition, the second equipped STM SPECS Aarhus 150 SPECS SPC 260 controller, both with Ar^+ sputtering tip cleaning[10]. STM with constant current[10].

CONCLUSION

The experiments were performed at different temperatures 400-500 K demonstrated the honeycomb at 420 K as more stable, less dense and a highly organized MoF.
The Theoretical approach show that Cu-N binding energies with PBE 1.56 eV, and 2.68 eV with PBE-D3, and molecule binding energy to the slab 6.71 eV for PBE, and 14.10 for PBE-D3.
This work demonstrates MoFs with a pore size of approx. 13 nm[2].

References

Acknowledgements

Thanks to the School of Physical and Nanotechnology, Yachay Tech University, who supported with computational cluster Imbabura.
Thanks to IFGW, UNICAMP, who supported in the performance of the experiments.

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