PÔSTER - RESUMO - DISPOSITIVOS ELETRÔNICOS, ELETROQUÍMICOS, SUPERCAPACITORES E BATERIAS

# INVESTIGATION OF CHARGE TRANSPORT MECHANISMS IN HYBRID QUANTUM MATERIALS

*Kemyle Carvalho Cassu Alves (kemyle.cassu@unesp.br)*

*Carlos César Bof Bufon (cesar.bof@unesp.br)*

Hybrid organic–inorganic materials have emerged as strategic platforms for electronics and sensing by combining structural modularity, chemical functionalization, and tunable physicochemical properties [1]. Among these systems, Metal–Organic Frameworks (MOFs) stand out as porous crystalline networks composed of metal nodes and organic linkers, exhibiting high surface area and chemical tunability [2].

One of the most extensively studied MOFs is HKUST-1 (Cu3(BTC)2), which consists of Cu²? paddle-wheel dimers interconnected by 1,3,5-benzenetricarboxylate linkers. The presence of unsaturated metal sites and high affinity for polar molecules enables applications in gas storage and separation, catalysis, and sensors based on adsorption-induced conductivity modulation [3].

In this work, HKUST-1 thin films were synthesized via robotic layer-by-layer (LbL) deposition by liquid-phase epitaxy (LPE), enabling controlled, oriented film growth. Deposition was performed on alumina and SiO2 chips containing platinum interdigitated electrodes, allowing precise control of film thickness, homogeneity, and surface coverage by adjusting the number of deposition

cycles, exposure time, and precursor concentration. This strategy yielded continuous and adherent films suitable for planar electrical characterization.

Electrical response was investigated through current–voltage (I×V) measurements at room temperature under different relative humidity (RH) levels. In general, humidity influences the electrical conduction of the films, suggesting that the adsorption of water molecules within the pores and at metal sites may affect charge-transport mechanisms. This behavior is consistent with adsorption-assisted conduction and potential barrier modifications within the material. Complementary electrical impedance spectroscopy (EIS) measurements were performed as a function of frequency and humidity, also at room temperature. Preliminary analysis indicates that humidity exerts a measurable influence on the system's overall electrical response, possibly involving resistive and capacitive contributions from the material and electrode/film interfaces. These results are currently under analysis to elucidate the underlying transport dynamics.

Raman spectroscopy confirmed the structural integrity of HKUST-1 after thin-film growth, as evidenced by characteristic vibrational modes of the BTC linker and Cu–O bonds, with no indication of secondary phases.

In summary, HKUST-1 thin films prepared via LbL–LPE and integrated with interdigitated electrodes constitute a robust platform for investigating charge-transport mechanisms in humidity-sensitive MOFs. The observed dependence of conductivity on water adsorption motivates further studies to distinguish the relative contributions of electronic hopping, ionic (protonic) conduction, and mixed transport mechanisms. Beyond sensing applications, these films also show potential for resistive memory devices, such as memristors, based on reversible resistance modulation induced by adsorption and species migration within the porous framework.

Acknowledgments: The authors acknowledge financial support from the Fundação de Amparo à Pesquisa do Estado de São Paulo (Grant No. 2025/27044-5), the Conselho Nacional de Desenvolvimento Científico e Tecnológico (Grant No. 408449/2024-1), and the Instituto Nacional de Eletrônica Orgânica e Sustentável (INEO).

[1] GOMEZ-ROMERO, Pedro; POKHRIYAL, Anukriti; RUEDA-GARCÍA, Daniel; BENGOA, Leandro N.; GONZÁLEZ-GIL, Rosa M. Hybrid Materials: A Metareview. Chemistry of Materials, v. 36, n. 1, p. 8–27, 2023. DOI: https://doi.org/10.1021/acs.chemmater.3c01878

[2] OHARA, Hiroaki; YAMAMOTO, Shunsuke; KUZUHARA, Daiki; KOGANEZAWA, Tomoyuki; OIKAWA, Hidetoshi; MITSUISHI, Masaya. Layer-by-layer growth control of metal–organic framework thin films assembled on polymer films. ACS Applied Materials & Interfaces, v. 12, n. 45, p. 50784–50792, 2020. DOI: https://doi.org/10.1021/acsami.0c13016

[3] ZHAO, Tian; NIE, Saiqun; LUO, Mingliang; XIAO, Ping; PENGCHENG, Xiao; ZOU, Mijun; ZOU, Minmin; CHEN, Yi; CHEN, Yi. Research progress in structural regulation and applications of HKUST-1 and HKUST-1 based materials. Journal of Alloys and Compounds, v. 974, p. 172897, 2024. DOI: https://doi.org/10.1016/j.jallcom.2023.172897

Palavras-chave: materiais híbridos; hkust-1; transporte de carga.