

Molecular and electrochemical doping in organic and metal-organic materials

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Physical properties of molecules change drastically as results of interactions with surrounding environments. For instance, encapsulation into a hosting material having a large band gap allows molecules to be electronically isolated, while covalent bonding and charge transfer to hosting sites can alter properties of the host. In our recent study [1] 7,7,8,8-tetracyanoquinodimethane (TCNQ) was encapsulated into a crystal of melamine. Combined mass spectrometry, fluorescence excitation-emission spectral mapping, and density-functional theory (DFT) calculations demonstrated that the TCNQ, which is barely luminescent in its solid state, becomes a bright luminophore in crystalline melamine. On the contrary, molecular and electrochemical doping in metal-organic frameworks (MOFs) offer means for changing the properties of the framework. MOFs whose optical properties change upon redox reactions have great potential as multifunctional elements in optoelectronics. In Ref [2], using spectroelectrochemistry which combines electrochemistry and optical spectroscopy we show that NU-1000, a redox-active zirconium pyrenetetra benzoate MOF, exhibits both electrochromism and electrofluoreochromism. DFT calculations suggest the singly-occupied molecular orbital (SOMO) of the radical linker responsible for the fluorescence quenching in the oxidized NU-1000.

[1] V. Mishra, A. Mantel, P. Kapusta, A. Prado-Roller, H. Shiozawa "Highly luminescent TCNQ in melamine" <https://doi.org/10.26434/chemrxiv-2023-945vj>.

[2] A. El Guerraf, W. Zeng, A. Mantel, E. H. Benhsina, J. M. Chin, H. Shiozawa "Synchronous electrochromism and electrofluorochromism in a zirconium pyrenetetra benzoate metal-organic framework" <https://doi.org/10.26434/chemrxiv-2023-6c07v>.