2023 Helmholtz – OCPC – Programme

for the involvement of postdocs in bilateral collaboration projects

PART A

Title of the project:

Virtual design of the optoelectronic properties of metal organic frameworks

Helmholtz Centre and/or institute:

Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology (INT)

Project leader:

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Description of the project (max. 1 page)**:**

Metal-organic frameworks (MOF) are a class of nanoporous designer materials where the individual building blocks, namely metal clusters, also known as secondary building units (SBUs), and organic linkers, can be chosen from a combinatorial list of options to build crystalline assemblies with many interesting properties. Crystals of particularly high quality can be assembled using the layer-by-layer technique for SURMOF synthesis, which involves alternating deposition and rinsing cycles to stack 2D layers aligned in the x-y plane upon one another, iteratively thickening the SURMOF in the z-direction to maintain high degree of alignment and defect suppression with unprecedented spatio-temporal control over the growth.[1,2]

In collaboration with the local experimental group of Prof. Christof Wöll (https://www.ifg.kit.edu/english/21_264.php) we have in recent years developed a multiscale

simulation techniques[3] to investigate a number of fascinating electrooptical properties in metal organic frameworks, including charge transport[4,5], design of the phosphorescence properties[6] spontaneous self-organization of the linkers[7]. We propose here to continue the latter project to design linkers with an improved propensity to self-organize with respect to their orientation in the growth phase. In prior work we have been able to establish basic principles of the underlying mechanisms, but many questions remain open. In addition, we would like to MOF with improved electrical conductivity, either by linker design or by the implementation of doping strategies.

(1) Chen, D.-H.; Gliemann, H.; Wöll, C. Layer-by-Layer Assembly of Metal-Organic Framework Thin Films: Fabrication and Advanced Applications. *Chem. Phys. Rev.* **2023**, *4* (1), 011305. https://doi.org/10.1063/5.0135019.

(2) Zhang, Q.; Pramudya, Y.; Wenzel, W.; Wöll, C. Modeling the Layer-by-Layer Growth of HKUST-1 Metal-Organic Framework Thin Films. *Nanomaterials* **2021**, *11* (7), 1631. https://doi.org/10.3390/nano11071631.

(3) Mostaghimi, M.; Rego, C.; Haldar, R.; Woll, C.; Wenzel, W.; Kozlowska, M. Automated Virtual Design of Organic Semiconductors Based on Metal-Organic Frameworks. *FRONTIERS IN MATERIALS* **2022**, *9*. https://doi.org/10.3389/fmats.2022.840644.

(4) Liu, X.; Kozlowska, M.; Okkali, T.; Wagner, D.; Higashino, T.; Brenner-Weifss, G.; Marschner, S. M.; Fu, Z.; Zhang, Q.; Imahori, H.; Braese, S.; Wenzel, W.; Woell, C.; Heinke, L. Photoconductivity in Metal-Organic Framework (MOF) Thin Films. *Angew. Chem.-Int. Edit.* **2019**, *58* (28), 9590–9595. https://doi.org/10.1002/anie.201904475.

(5) Garg, S.; Schwartz, H.; Kozlowska, M.; Kanj, A. B.; Müller, K.; Wenzel, W.; Ruschewitz, U.; Heinke, L. Conductance Photoswitching of Metal–Organic Frameworks with Embedded Spiropyran. *Angewandte Chemie International Edition* **2019**, *58* (4), 1193–1197. https://doi.org/10.1002/anie.201811458.

(6) Haldar, R.; Mazel, A.; Krstić, M.; Zhang, Q.; Jakoby, M.; Howard, I. A.; Richards, B. S.; Jung, N.; Jacquemin, D.; Diring, S.; Wenzel, W.; Odobel, F.; Wöll, C. A de Novo Strategy for Predictive Crystal Engineering to Tune Excitonic Coupling. *Nat Commun* **2019**, *10* (1), 2048. https://doi.org/10.1038/s41467-019-10011-8.

(7) Nefedov, A.; Haldar, R.; Xu, Z.; Kühner, H.; Hofmann, D.; Goll, D.; Sapotta, B.; Hecht, S.; Krstić, M.; Rockstuhl, C.; Wenzel, W. Avoiding the Center-Symmetry Trap: Programmed Assembly of Dipolar Precursors into Porous, Crystalline Molecular Thin Films. *Advanced Materials* **2021**. https://doi.org/doi.org/10.1002/adma.202103287.

Description of existing or sought Chinese collaboration partner institute (max. half page)**:**

Tackling these problems involves the combination of several simulation techniques, pertaining to the electronic structure of the linkers and the metal organic framework (mostly DFT and TD-DFT) in combination with methods to simulate the structure, dynamics and the growth process of metal organic frameworks (molecular dynamics, and ab-initio molecular dynamics). Given the large number of metal organic frameworks that have been realized (>100.000) and that are potentially realizable (>4.000.000) the development of computational high throughput techniques is highly desirable.

Required qualification of the postdoc:

- PhD in Theoretical Chemistry or Theoretical Physics
- Experience with electronic structure calculations in molecular crystals or molecular aggregates
- Additional skills in molecular dynamics, python programming
- Language requirement: English

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