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RESEARCH INTERESTS

- Nanoporous materials (Metal-Organic Frameworks, Zeolites,)
- Photocatalysis and CO_2 reduction
- Computational chemistry and crystal structure prediction
- Surface chemistry, gas adsorption and separation
- "Host-guest" interactions

SUMMARY

My research interests concern the computational chemistry of crystalline materials and the understanding of structure-properties relationships, in close conjunction with parallel experimental investigations. My research efforts relate to nanoporous materials (zeolites, hybrid organic-inorganic frameworks, MOFs, POMOFs) as tunable platforms to perform adsorption/separation processes, catalysis and photocatalysis. We use molecular level modeling, including both ab initio and force-field approaches, to gain a deeper insight into the atomic scale structure of existing or hypothetical crystalline edifices, with a special attention to what might induce specific properties, stabilize specific structures (template, organic linkers, linker's substituents) and destabilize others, while elucidating processes occurring at the host-guest interface. With respect to metal-organic frameworks, a recent focus is to develop strategies for targeting new photocatalytic systems by taking advantage of MOFs modular nature to heterogenize and stabilize efficient molecular catalysts for the photoreduction of CO_2. I also explore the computational design of bio-inspired materials combining MOFs' porosity and enzymatic functionalities imported through the grafting of amino acids, and explore host-guest interactions using combined simulated annealing and Density Functional Theory calculations.

PUBLICATIONS

Selected Publications

- Immobilization of a full photosystem in the large pore MIL-101 Metal-organic Framework for CO_2 reduction. X. Wang, F. M. Wisser, J. Canivet, M. Fontecave, **C. Mellot-Draznieks** (2018) *ChemSusChem*. 11, 3315-3322
- Encoding evolution of porous solids. **Mellot-Draznieks C** & Cheetham AK. (2017) *Nature Chemistry* 9:6-8.

- Maximizing the Photocatalytic Activity of Metal-Organic Frameworks with Aminated-Functionalized Linkers: Substoichiometric Effects in MIL-125-NH_2. Chambers, MB; Wang, X; Ellezam, L; Ersen, O; Fontecave, M; Sanchez, C; Rozes, L; Mellot-Draznieks, C. (2017). *J. Amer. Chem. Soc.* 139,4, 8222-8228.
- Photocatalytic Carbon Dioxide Reduction with Rhodium-based Catalysts in Solution and Heterogenized within Metal-Organic Frameworks. Chambers MB, Wang X, Elgrishi N, Hendon CH, Walsh A, Bonnefoy J, Canivet J, Quadrelli EA, Farrusseng D, **Mellot-Draznieks C**, Fontecave M. *ChemSusChem.* 2015, 8, 603-608.
- Engineering the Optical Response of the Titanium-MIL-125 Metal-Organic Framework through Ligand Functionalization. Hendon CH, Tiana, D, Fontecave M, Sanchez C, D'Arras L, Sassoye C, Rozes L, **Mellot-Draznieks C**, Walsh A. *J. Am. Chem. Soc.* 2013, 135, 10942-10945.
- Impact of functionalized linkers on the energy landscape of ZIFs. Galvelis, Slater B, Chaudret R, Creton B, Nieto-Draghi C, **Mellot-Draznieks. C**. *CrystEngComm.* 2013, 15, 9603-9612.
- Functionalized MOFs for enhanced CO_2 capture. Torrisi A, Bell Rg, **Mellot-Draznieks C.** *Crystal Growth and Design* 2010, 10, 2839-2841.
- Zeolitic polyoxometalate-based metal-organic frameworks (Z-POMOFs): computational evaluation of hypothetical polymorphs and the successful targeted synthesis of the redox-active Z-POMOF1. Rodriguez-Albelo LM, Ruiz-Salvador AR, Sampieri A, Lewis DW, Gómez A, Nohra B, Mialane P, Marrot J, Sécheresse F, **Mellot-Draznieks C**, Ngo Biboum R, Keita B, Nadjo L, Dolbecq A. *J. Am. Chem. Soc.* 2009, 131, 16078-87.
- A chromium terephthalate-based solid with unusually large pore volumes and surface area. Férey G, **Mellot-Draznieks C**, Serre C, Millange F, Dutour J, Surblé S, Margiolaki I. *Science***,** 2005, 309, 2040-2.

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- Structure-directing role of immobilized polyoxometalates in the synthesis of porphyrinic Zr-based Metal-Organic Frameworks. M. Duguet, A. Lemarchand, Y. Benseguir, P. Mialane, M. Gomez-Mingot, C. Roch, M. Haouas, M. Fontecave, **C. Mellot-Draznieks**, C. Sassoye, A. Dolbecq *Chem. Commun.* 2020, 56, 10143-10146.
- Synthetic and computational assessment of a chiral metal–organic framework catalyst for predictive asymmetric transformation. J. Canivet, E. Bernoud, J. Bonnefoy, A. Legrand, T. K. Todorova, E. A. Quadrelli, **C. Mellot-Draznieks** *Chem. Sci.* 2020, 11, 8800-8808 DOI: 10.1039/d0sc03364b.
- Co-immobilization of a Rh Catalyst and a Keggin Polyoxometalate in the UiO-67 Zr-Based Metal-Organic Framework: In Depth Structural Characterization and Photocatalytic Properties for CO_2 Reduction. Y. Benseghir, A. Lemarchand, M. Duguet, Pierre Mialane, Maria Gomez-Mingot, C. Roch-Marchal, T. Pino, M.-H. Ha-Thi, M. Haouas, M. Fontecave, A. Dolbecq, C. Sassoye, **C. Mellot-Draznieks** *J. Am. Chem. Soc.* 2020, 142, 20, 9428–9438.
- Molecular Porous Photosystems Tailored for Long-Term Photocatalytic CO_2 Reduction. F. M. Wisser, M. Duguet, Q. Perrinet, A. C. Ghosh, M. Alves-Favaro, Y. Mohr, C. Lorentz, E. A. Quadrelli, R. Palkovits, D. Farrusseng, **C. Mellot-Draznieks**, V. De Waele, J. M. Canivet *Angew. Chem. Int. Ed.* 2020, 59, 5116-5122.

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- An unprecedented $\{Ni_{14}SiW_9\}$ hybrid polyoxometalate with high photocatalytic hydrogen evolution activity. G. Paille, A. Boulmier, A. Bensaid, M. H. Ha-Thi; T. G. Tran, T. Pino, J. Marrot, E. Riviere, C. H. Hendon, O. Oms, M. Gomez-Mingot, M. Fontecave, **C. Mellot-Draznieks**, A. Dolbecq, P. Mialane. *Chem. Comm.* **2019**, 55, 29, 4166-4169.
- Thin Films of Fully Noble Metal-Free POM@MOF for Electrocatalytic and Photocatalytic Water Oxidation. G. Paille, M. Gomez-Mingot, C. Roch-Marchal, M. Haouas, Y. Benseghir, Thomas Pino, M.-H. Ha-Thi, G. Landrot, P. Mialane, M. Fontecave, A. Dolbecq, **C. Mellot-Draznieks** (Submitted)

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- Immobilization of a full photosystem in the large pore MIL-101 Metal-organic Framework for CO_2 reduction. X. Wang, F. M. Wisser, J. Canivet, M. Fontecave, **C. Mellot-Draznieks** (2018) *ChemSusChem*. 11, 3315-3322.
- Novel Ni-IRMOF-74 Postsynthetically Functionalized for H_2 Storage Applications. H. Monte-Andres, G. Orcajo, **C. Mellot-Draznieks**, C. Martos, J. A.. Botas, G. Calleja. (2018) *J. Phys. Chem. C* 122, 49, 28123-28132.
- A Fully Noble Metal-Free Photosystem Based on Cobalt-Polyoxometalates Immobilized in a Porphyrinic Metal-Organic-Framework for Water Oxidation. G. Paille, M. Gomez-Mingot, C. Roch-Marchal, B. Lassalle-Kaiser, P. Mialane, M. Fontecave, **C. Mellot-Draznieks**, A. Dolbecq (2018) *J. Am. Chem. Soc.* 140, 3613-3618.
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- Maximizing the Photocatalytic Activity of Metal-Organic Frameworks with Aminated-Functionalized Linkers: Substoichiometric Effects in MIL-125-NH_2. Chambers, MB; Wang, X; Ellezam, L; Ersen, O; Fontecave, M; Sanchez, C; Rozes, L; **Mellot-Draznieks, C.** (2017) *J. Amer. Chem. Soc.* 139,4, 8222-8228.
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