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### RESEARCH INTERESTS

- Nanoporous materials (Metal-Organic Frameworks, Zeolites,)
- Photocatalysis and CO<sub>2</sub> 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<sub>2</sub>. 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

- 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<sub>2</sub>. 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-Drazniaks 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, Sassoey C, Rozes L, **Mellot-Drazniaks 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-Drazniaks. C.** *CrystEngComm*. 2013, **15**, 9603-9612.
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  - 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-Drazniaks C**, Ngo Biboum R, Keita B, Nadjo L, Dolbecq A. *J. Am. Chem. Soc.* 2009, **131**, 16078-87.
  - Role of computer simulations in structure prediction and structure determination: from molecular compounds to hybrid frameworks. **C. Mellot-Drazniaks.** *J. Mater. Chem.* 2007, **17**, 4348-4358.
  - A chromium terephthalate-based solid with unusually large pore volumes and surface area. Férey G, **Mellot-Drazniaks C**, Serre C, Millange F, Dutour J, Surblé S, Margiolaki I. *Science*, 2005, **309**, 2040-2.

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- Encoding evolution of porous solids. Mellot-Drazniaks 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<sub>2</sub>. Chambers, MB; Wang, X; Ellezam, L; Ersen, O; Fontecave, M; Sanchez, C; Rozes, L; Mellot-Drazniaks, C. (2017) *J. Amer. Chem. Soc.* 139,4, 8222-8228.
- Effect of Cations on the Structure and Electrocatalytic Response of Polyoxometalate-Based Coordination Polymers. Salomon W, Paille G, Gomez-Mingot M, Mialane P, Marrot J, Roch-Marchal C, Nocton G, **Mellot-Drazniaks C**, Fontecave M, & Dolbecq A. (2017) *Crystal Growth & Design* **17**:1600-1609.
- Flexible Ligand-Based Lanthanide Three-Dimensional Metal-Organic Frameworks with Tunable Solid-State Photoluminescence and OH-Solvent-Sensing Properties. Gomez, GE; Brusau, EV; Kaczmarek, AM; Mellot-Drazniaks, C; Sacanell, J; Rouse, G; Van Deun, R; Sanchez, C ; Narda, GE; Illia, GJAAS. (2017) *European Journal of Inorganic Chemistry*, 17, 2321-2331.
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