

## Dr Caroline Mellot-Draznieks

### (DR1 CNRS, HDR)

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### RESEARCH INTERESTS

- Nanoporous materials (Metal-Organic Frameworks, Zeolites,)
- Photocatalysis (CO<sub>2</sub> reduction, water oxidation)
- Computational chemistry and crystal structure prediction
- Surface chemistry, gas adsorption and separation
- “Host-guest” interactions

### SUMMARY OF ACADEMIC APPOINTMENTS

<u>Collège de France, Paris</u>	
Director of Research-CNRS	2011-present
<u>University College London, UK</u>	
EPSRC Advanced Research Fellow at UCL	2007-2011
Visiting Scientist at IFPEN, Rueil-Malmaison, France	2009-2011
<u>Royal Institution, London, UK</u>	
CNRS Research Fellow at the RI	2005-2007
<u>University of Versailles, France</u>	
CNRS Research Fellow	1998-2005
Post-doctoral Researcher	1997-1998
<u>University of California, Santa Barbara, USA</u>	
Post-doctoral Researcher, Lavoisier Fellowship	1996-1997
<u>L’AIR LIQUIDE, R&amp;D Research Centre, Jouy-en-Josas, France</u>	
Research Engineer	1993-1996

### SUMMARY OF EDUCATION

<u>Ecole Normale Supérieure (ENS-Ulm) Paris</u>	1988-1992
<u>PhD in Materials Chemistry ,Université Pierre et Marie Curie/IFPEN</u>	1990-1993

### PUBLICATIONS

#### Selected Publications

- Heterogenized Molecular Rhodium Phosphine Catalysts within Metal–Organic Frameworks for Alkene Hydroformylation. P. Samanta, A. Solé-Daura, Remy Rajapaksha, Florian M. Wisser, F. Meunier, Y. Schuurman, C. Sassoie, **C. Mellot-Draznieks**, J. Canivet. (2023) *ACS Catal.* 13, 7, 4193–4204.
- Unveiling the mechanism of the photocatalytic reduction of CO<sub>2</sub> to formate promoted by porphyrinic Zr-based metal–organic frameworks. Y. Benseghir, A. Solé-Daura, D. Cairnie, A. Robinson, M. Duguet, P. Mialane, P. Gairola, M. Gomez-Mingot, M. Fontecave, D. Iovan, B.

- Bonnett, A. J. Morris, A. Dolbecq, **C. Mellot-Draznieks**. (2022) *J. Mater. Chem. A*, 10 (35), pp.18103-18115.
- Origin of the Boosting Effect of Polyoxometalates in the Photocatalysis: the case of CO<sub>2</sub> Reduction by a Rh-Containing Metal-Organic Framework. A. Solé-Daura, Y. Benséghir, M.-H. Ha-Thi, M. Fontecave, P. Mialane, A. Dolbecq, **C. Mellot-Draznieks**. (2022) *ACS Catalysis*, 12, 9244-9255.
  - 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<sub>2</sub> 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. Sassoys, **C. Mellot-Draznieks** *J. Am. Chem. Soc.* 2020, 142, 20, 9428–9438.
  - 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.
  - 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, Sassoys C, Rozes L, **Mellot-Draznieks C**, Walsh A. *J. Am. Chem. Soc.* 2013, 135, 10942-10945.

**All publications** (Web of Science Query: mellot-draznieks or draznieks or mellot c\*) h index = 50

#### 2023

- Unravelling the Molecular Structure and Confining Environment of an Organometallic Catalyst Heterogenized within Amorphous Porous Polymers. R. Jabbour, C.W. Ashling, T.C. Robinson, A.H. Khan, D. Wisser, P. Berruyer, A.C. Ghosh, A. Ranscht, D.A. Keen, E. Brunner, J. Canivet, TD Bennett, **C. Mellot-Draznieks**, A. Lesage, F.M. Wisser. (2023) *Angew. Chem. Int. Ed.* 62, 44, e202310878.
- Controlled Growth of a Photocatalytic Metal–Organic Framework on Conductive Plates by Mixing Direct Synthesis and Postsynthetic Modification Strategies. G. Genesio, B. Mortada, A.L. Robinson, J. Maynadié, M. Odorico, **C. Mellot-Draznieks**, M. Fontecave, M. Carboni, D. Meyer (2023) *ACS Appl. Energy Mater.* 6, 18, 9188–9195.
- Heterogenized Molecular Rhodium Phosphine Catalysts within Metal–Organic Frameworks for Alkene Hydroformylation. P. Samanta, A. Solé-Daura, Remy Rajapaksha, Florian M. Wisser, F. Meunier, Y. Schuurman, C. Sassoys, **C. Mellot-Draznieks**, J. Canivet. (2023) *ACS Catal.* 13, 7, 4193–4204.
- ZIF-8 thin films by a vapor-phase process: limits to Growth. V. Perrot, A. Roussey, A. Benayad, M. Veillerot, D. Mariolle, A. Solé-Daura, **C. Mellot-Draznieks**, F. Ricoul, J. Canivet, E. A. Quadrelli, V. Jousseau. (2023) *Nanoscale*, 2023, 15, 7115

#### 2022

- Understanding the Photocatalytic Reduction of CO<sub>2</sub> with Heterometallic Molybdenum(V) Phosphate Polyoxometalates in Aqueous Media. Y. Benséghir, A. Solé-Daura, P. Mialane, J. Marrot, L. Dalecky, S. Bechu, M. Fregnaud, M. Gomez-Mingot, M. Fontecave, **C. Mellot-Draznieks**, A. Dolbecq. (2022) *ACS Catalysis*, 12, 453-464.
- Origin of the Boosting Effect of Polyoxometalates in the Photocatalysis: the case of CO<sub>2</sub> Reduction by a Rh-Containing Metal-Organic Framework. A. Solé-Daura, Y. Benséghir, M.-H. Ha-Thi, M. Fontecave, P. Mialane, A. Dolbecq, **C. Mellot-Draznieks**. (2022) *ACS Catalysis*, 12, 9244-9255.
- Unveiling the mechanism of the photocatalytic reduction of CO<sub>2</sub> to formate promoted by porphyrinic Zr-based metal–organic frameworks. Y. Benseghir, A. Solé-Daura, D. Cairnie, A. Robinson, M. Duguet, P. Mialane, P. Gairola, M. Gomez-Mingot, M. Fontecave, D. Iovan, B. Bonnett, A. J. Morris, A. Dolbecq, **C. Mellot-Draznieks**. (2022) *J. Mater. Chem. A*, 10 (35), pp.18103-18115.
- Heterogenization of molecular cobalt catalysts in robust metal-organic frameworks for efficient photocatalytic CO<sub>2</sub> reduction. S. Parshamoni, C. Vivaraux, M. Robert, **C. Mellot-Draznieks**, G. Chen, P. Mialane, A. Dolbecq, J. Bonin. (2022) *Catal. Sci & Tech.* 12, pp. 5418-5424.

- Electrocatalytic Conversion of CO<sub>2</sub> to Formate at Low Overpotential by Electrolyte Engineering in Model Molecular Catalysis. E. Vichou, A. Sole-Daura, **C. Mellot-Draznieks**, Y. Li, M. Gomez-Mingot, M. Fontecave, C. M. Sanchez-Sanchez. *ChemSusChem*. 2022, 15, e202201566.

## 2021

- Heterogenization of a Molecular Ni Catalyst within a Porous Macroligand for the Direct C-H Arylation of Heteroarenes. Y. Mohr, M. Alves-Favaro, R. Rajapaksha, G. Hisler, A. Ranscht, P. Samanta, C. Lorentz, M. Duguet, **C. Mellot-Draznieks**, A.E. Quadrelli, F. M. Wisser, J. Canivet. (2021) *ACS Catal.* 11, 3507-3515.
- Heterogenisation of polyoxometalates and other metal-based complexes in metal-organic frameworks: from synthesis to characterisation and applications in catalysis. P. Mialane, **C. Mellot-Draznieks**, P. Gairola, M. Duguet, Y. Benseghir, O. Oms, A. Dolbecq. (2021) *Chem. Soc. Rev.* 50, 6152-6220.
- Temperature sensors based on europium polyoxometalate and mesoporous terbium metal-organic framework. C. Viravaux, O. Oms, A. Dolbecq, E. Nassar, L. Busson, **C. Mellot-Draznieks**, R. Dessapt, H. Serier-Brault, P. Mialane. (2021) *J. Mater. Chem.* 9 (26) 8323-8328.
- Impact of organic templates on the selective formation of zeolite oligomers. M. Ciantar, T. T. Trinh, C. Michel, P. Sautet, **C. Mellot-Draznieks**, C. Nieto-Draghi. (2021) *Angew. Chem. Int. Ed.* 60 (13) 7111-7116.

## 2020

- Structure-directing role of immobilized polyoxometalates in the synthesis of porphyrinic Zr-based Metal-Organic Frameworks. M. Duguet, A. Lemarchand, Y. Benseghir, P. Mialane, M. Gomez-Mingot, C. Roch, M. Haouas, M. Fontecave, **C. Mellot-Draznieks**, C. Sassoey, 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<sub>2</sub> 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. Sassoey, **C. Mellot-Draznieks** *J. Am. Chem. Soc.* 2020, 142, 20, 9428-9438.
- Molecular Porous Photosystems Tailored for Long-Term Photocatalytic CO<sub>2</sub> 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 .

## 2019

- An unprecedented {Ni<sub>14</sub>SiW<sub>9</sub>} 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** *ACS Applied Materials & Interfaces*, 11, 47837-47845.

## 2018

- Immobilization of a full photosystem in the large pore MIL-101 Metal-organic Framework for CO<sub>2</sub> 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<sub>2</sub> 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.

- A Bioinspired Nickel(bis-dithiolene) Complex as a Novel Homogeneous Catalyst for Carbon Dioxide Electroreduction . T. Fogeron, T. K. Todorova, J.-P. Porcher, M. Gomez-Mingot, L.-M. Chamoreau, **C. Mellot-Draznieks**, Y. Li, M. Fontecave (2018) *ACS Catalysis*, 8, 2030-2038.

## 2017

- 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.
- 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-Draznieks 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-Draznieks, C**; Sacanell, J; Rouse, G; Van Deun, R; Sanchez, C ; Narda, GE; Illia, GJAAS. (2017) *European Journal of Inorganic Chemistry*, 17, 2321-2331.
- Tackling the Defect Conundrum in UiO-66: A Mixed-Linker Approach to Engineering Missing Linker Defects. B. Bueken, N. Van Velthoven, A. Krajnc, S. Smolders, F. Taulelle, **C. Mellot-Draznieks**, G. Mali, T. D. Bennett, D. de Vos (2017) *Chem. Mater.* 29, 10478-10486
- The UbiK protein is an accessory factor necessary for bacterial ubiquinone (UQ) biosynthesis and forms a complex with the UQ biogenesis factor UbiJ. Loiseau, L; Fyfe, C; Aussel, L; Chehade, MH; Hernandez, SB; Faivre, B; Hamdane, D; **Mellot-Draznieks, C**; Rascalou, B; Pelosi, L ; Velours, C; Cornu, D; Lombard, M; Casadesus, J ; Pierrel, F; Fontecave, M; Barras, F. (2017) *J. Biol. Chem.* 292, 28, 11937-11950.

## 2016

- Molecular Level Characterization of the Structure and Interactions in Peptide-Functionalized Metal-Organic Frameworks. Todorova TK, Rozanska X, Gervais C, Legrand A, Ho LN, Berruyer P, Lesage A, Emsley L, Farrusseng D, Canivet J, & **Mellot-Draznieks C.** (2016) *Chemistry - A European Journal* 22:16531-16538.
- Connecting defects and amorphization in UiO-66 and MIL-140 metal-organic frameworks: a combined experimental and computational study. Bennett, TD; Todorova, TK; Baxter, E.; Reid, DG; Gervais, C; Bueken, B; Van de Voorde, B; De Vos, D; Keen, DA ; **Mellot-Draznieks, C.** (2106) *Phys. Chem. Chem. Phys.* 18, 3, 2192-2201.
- Réduction du CO<sub>2</sub> dans des matériaux à charpentes hybrides : contrôle de l'absorption de lumière et incorporation de catalyseurs moléculaires. Paille G, Fontecave M, & **Mellot-Draznieks C.** (2016) *L'actualité chimique* 408-409:64-67.
- A Simple and Non-Destructive Method for Assessing the Incorporation of Bipyridine Dicarboxylates as Linkers within Metal-Organic Frameworks. Hendon CH, Bonnefoy J, Quadrelli EA, Canivet J, Chambers MB, Rouse G, Walsh A, Fontecave M, & **Mellot-Draznieks C.** (2016) *Chemistry - A European Journal* 22:3713-3718.
- A cobalt complex with a bioinspired molybdopterin-like ligand: a catalyst for hydrogen evolution. Fogeron T, Porcher J-P, Gomez-Mingot M, Todorova TK, Chamoreau L-M, **Mellot-Draznieks C**, Li Y, & Fontecave M. (2016) *Dalton Transactions* (Cambridge, England: 2003) 45:14754-14763.
- Coenzyme Q Biosynthesis: Evidence for a Substrate Access Channel in the FAD-Dependent Monooxygenase Coq6. Ismail, A ; Leroux, V; Smadja, M; Gonzalez, L; Lombard, M ; Pierrel, F ; **Mellot-Draznieks, C.**; Fontecave, M. (2016) *PLOS Computational Biology*, 12,1, e1004690.

## 2015

- 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.

- Computational exploration of metal–organic frameworks: examples of advances in crystal structure predictions and electronic structure tuning. **Mellot-Draznieks C.** (2015) *Molecular Simulation* 41:1422-1437.
- Extreme Flexibility in a Zeolitic Imidazolate Framework: Porous to Dense Phase Transition in Desolvated ZIF 4. Wharmby MT, Henke S, Bennett TD, Bajpe SR, Schwedler I, Thompson SP, Gozzo F, Simoncic P, **Mellot-Draznieks C**, Tao H, Yue Y, Cheetham AK (2015) *Angew. Chemie Int. Ed.* 54, 22, 6447-6451.
- A Kinetic Monte Carlo Simulation Study of Synthesis Variables and Diffusion Coefficients in Early Stages of Silicate Oligomerization. Ciantar, M; **Mellot-Draznieks, C**; Nieto-Draghi, C. (2015) *J. Phys. Chem. C*, 119, 52, 28871-28884.
- Bioinspired Tungsten Dithiolene Catalysts for Hydrogen Evolution: A Combined Electrochemical, Photochemical and Computational Study. Gomez-Mingot M, Porcher JP, Todorova T; Forgeron T, **Mellot-Draznieks C**; Li Y, Fontecave M. (2015) *J. Phys. Chem. B*, 119, 43, 13524-13533.
- Coq6 Is Responsible for the C4-deamination Reaction in Coenzyme Q Biosynthesis in *Saccharomyces cerevisiae*. Ozeir, M; Pelosi, L; Ismail, A; Mellot-Draznieks, C; Fontecave, M; Pierrel, F (2015) *Journal of Biological Chemistry*, 290, 40, 24140-24151.

#### 2014

- Exploring the interplay between ligand and topology in zeolitic imidazolate frameworks with computational chemistry. **Mellot-Draznieks C**, Kerkeni B, **Molecular Simulation**, 2014, 40, 25-32.
- Photochemical reduction of CO<sub>2</sub> via heterogenization of catalysts within metal-organic frameworks: Evaluation of catalytic performance and light absorption strategies. Chambers MB, Wang X, Elgrishi N, **Mellot-Draznieks C**, Fontecave M. *Abstract of Papers of the American Chemical Society*, 2014, 248, 81-INOR.

#### 2013

- Solid State and Solution Mediated Multistep Sequential Transformations in Metal-Organic Coordination Networks. Mahata P, **Mellot-Draznieks C**, Roy P, Natarajan S. *Crystal Growth and Design*, 2013, 13, 155-168.
- 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.
- Functional and electrophysiological characterization of 4 non-truncating mutations responsible for creatine transporter deficiency syndrome. Valayannopoulos V, Bakouh N, Mazzuca M, Nonnemacher L, Hubert L, Makaci FL, Chabli A, Salomons GS, **Mellot-Draznieks C**, Brule E, de Lonlay P, Toulouhat H, Munnich A, Planelles G, de Keyser Y. *Journal of Inherited Metabolic Disease*, 2013, 36, 103-112.
- Predicting the impact of functionalized ligands on CO<sub>2</sub> adsorption in MOFs: A combined DFT and Grand Canonical Monte Carlo study. Torrisi A, Bell RG, **Mellot-Draznieks C.** *Microporous and mesoporous materials*, 2013, 168, 225-238.
- An NMR-Driven Crystallography Strategy to Overcome the Computability Limit of Powder Structure Determination: A Layered Aluminophosphate Case. Bouchevreau B, Martineau C, **Mellot-Draznieks C**, Tuel A, Suchomel MR, Trebosc J, Lafon, Amoureux JP, Taulelle F. *Chemistry, A European Journal*, 2013, 19, 5009-5013.
- High-Resolution Structural Characterization of Two Layered Aluminophosphates by Synchrotron Powder Diffraction and NMR Crystallographies. Bouchevreau B, Martineau C, **Mellot-Draznieks C**, Tuel A, Suchomel MR, Trebosc J, Lafon, Amoureux JP, Taulelle F. *Chemistry of Materials*, 2013, 25, 2227-2242.
- Ubil, a New Gene in *Escherichia coli* Coenzyme Q Biosynthesis, Is Involved in Aerobic C5-hydroxylation. Chehade MH, Loiseau L, Lombard M, Pecqueur L, Isamil A, Smadja M, Golinelli-Pimpaneau B, **Mellot-Draznieks C**, Hamelin O, Aussel L, Kieffer-Jaquinod S, Labessan N, Barras F, Fontecave M, Pierrel F. *Journal of Biological chemistry*, 2013, 288, 20085-20092.
- 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-Draznieks C**, Walsh A. *Journal of the American chemical Society*, 2013, 135, 10942-10945.

#### 2012

- Comparison of the relative stability of zinc and lithium-boron zeolitic imidazolate frameworks. Galvelis R, Slater B, Cheetham AK, **Mellot-draznieks C**, *CrystEngComm*. 2012,14, 374-378.
- Exceptionally Low Shear Modulus in a Prototypical Imidazole-Based Metal-Organic Framework. Tan JC, Civalleri B, Lin CC, Valenzano L, Galvelis R, Chen PF, Bennett TD, **Mellot-draznieks C**, Zicovich-wilson CM, Cheetham AK. *Phys Rev Lett*. 2012,108 :095502.

- Epsilon-Keggin-based coordination networks: Synthesis, structure and application toward green synthesis of polyoxometalate@graphene hybrids. Rodriguez-Albelo LM, Rousseau G, Mialane P, Marrot J, **Mellot-Draznieks C**, Ruiz-Salvador AR, Li SW, Liu RJ, Zhang GJ, Keita B, Dolbecq A. *Dalton Transactions*, 2012, 41, 9989-9999.
- Functional and electrophysiological characterization of 4 non-truncating mutations responsible for creatine transporter deficiency syndrome. Valayannopoulos V, Bakouh N, Mazzuca M, Nonnemacher L, Hubert L, Makaci FL, Chabli A, Salomons GS, **Mellot-Draznieks C**, Brule E, de Lonlay P, Toulouhat H, Munnich A, Planelles G, de Keyser Y. *Journal of Inherited Metabolic Disease*, 2012, 35, S54.
- Relative Enzymatic Activity Levels from In Silico Mutagenesis. **Mellot-Draznieks C**, Valayannopoulos V, Chretien D, Munnich A, de Lonlay P, Toulouhat H. *ACS Catalysis*, 2, 2673-2686.
- Flexibility and swing effect on the adsorption of energy-related gases on ZIF-8: combined experimental and simulation study. Fairen-Jimenez D, Galvelis R, Torrisi A, Gellan AD, Wharmby MT, Wright PA, **Mellot-Draznieks C**, Düren T. *Dalton Transactions*, 2012, 41, 10752-10762.

## 2011

- Thermodynamic methods and models to study flexible metal-organic frameworks. Coudert FX, Boutin A, Jeffroy M, **Mellot-Draznieks C**, Fuchs AH. *Chemphyschem*. 2011 Feb 7;12(2):247-58. doi: 10.1002/cphc.201000590.
- NMR crystallography of AlPO<sub>4</sub>-CJ2: from the topological network to the local (OH)/F distribution. Martineau C, **Mellot-Draznieks C**, Taulelle F. *Phys Chem Chem Phys*. 2011 Oct 28;13(40):18078-87.
- Polyoxometalate-based metal organic frameworks (POMOFs): structural trends, energetics, and high electrocatalytic efficiency for hydrogen evolution reaction. Nohra B, El Moll H, Rodriguez Albelo LM, Mialane P, Marrot J, **Mellot-Draznieks C**, O'Keefe M, Ngo Biboum R, Lemaire J, Keita B, Nadjó L, Dolbecq A. *J. Am Chem Soc*. 2011 Aug 31;133(34):13363-74.
- Clinical and biochemical heterogeneity associated with fumarase deficiency. Ottolenghi C, Hubert L, Allanore Y, Brassier A, Altzarra C, **Mellot-Draznieks C**, Bekri S, Goldenberg A, Veyrieres S, Boddaert N, Barbier V, Valayannopoulos V, Slama A, Chrétien D, Ricquier D, Marret S, Frebourg T, Rabier D, Munnich A, de Keyser Y, Toulouhat H, de Lonlay P. *Hum Mutat*. 2011 May 10; 32:1046-1052. doi: 10.1002/humu.21534.

## 2010

- Impact of ligands on CO<sub>2</sub> adsorption in metal-organic frameworks: First principles study of the interaction of CO<sub>2</sub> with functionalized benzenes. II. Effect of polar and acidic substituents. Torrisi A, **Mellot-Draznieks C**, Bell RG. *J Chem Phys*. 2010 Jan 28;132(4):044705.
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