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Full publication list

(updated 23rd August 2026)

Full publication list

In peer-reviewed international journals

178. "Systematic Study of Machine Learning Classification Algorithms of Zeolitic Imidazolate Framework Polymorphs", E. Méndez, L. Triestram, A. Dune, F.-X. Coudert and R. Semino, *J. Chem. Inf. Model.*, **2026**, in press.

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- "Preprints in the chemistry community", *ACS Fall 2021*, 22–26 August 2021, Atlanta (US) — held online.
- "Thermodynamic exploration of Xe/Kr separation", *Faraday Discussion on MOFs for Energy and the Environment*, 23–25 June 2021, Manchester (UK) — held online.
- "Responsive and disordered porous frameworks: connecting microscopic and macroscopic worlds", *MOF2020: 7th International Conference on Metal-Organic Frameworks and Open Framework Compounds*, 20–23 September 2020, Dresden (Germany) — held online.
- "Molecular simulation of soft porous crystals", *26th International Conference on Chemical Thermodynamics*, 19–23 July 2020, London (UK) — cancelled due to COVID-19.
- "The most flexible state of MOFs is the liquid!", *FlexMOF Symposium 2019*, 4–5 December 2019, Dresden (Germany).
- "Flexibility, defects and disorder in soft porous crystals", *Okinawa Colloids 2019*, 3–8 November 2019, Okinawa (Japan).
- "Soft Porous Crystals: Extraordinary Responses to Stimulation", *14th International conference on materials chemistry (MC14)*, 8–11 July 2019, Birmingham (UK).
- "Modelling Defects and Disorder in Nanoporous Materials", *MOFSIM 2019*, 10–12 April 2019, Ghent (Belgium).
- "Soft Porous Crystals: Extraordinary Responses to Stimulation", *MOF 2018*, 9–13 December 2018, Auckland (New Zealand).
- "Flexibility, defects and disorder in soft porous crystals", *SMARTER6*, 2–6 September 2018, Ljubljana (Slovenia).
- "Soft Porous Crystals: Extraordinary Responses to Stimulation", *Japanese Society of Coordination Chemistry*, 28–30 July 2018, Sendai (Japan).
- "Soft Porous Crystals: Extraordinary Responses to Stimulation", *GFZ International Congress*, 26–29 March 2018, Cabourg (France).

- "Soft Porous Crystals, Molecular Insight from Computational Chemistry", *Thermodynamics 2017*, 5–8 September 2017, Edinburgh (UK).
- "Flexibility, Defects & Disorder in Soft Porous Crystals", *7th FEZA Conference — Federation of European Zeolite Associations*, 3–7 July 2017, Sofia (Bulgaria).
- "Mechanical Impact of Adsorption in Compliant Nanoporous Materials", *Characterization of Porous Solids (COPS-XI)*, 14–17 May 2017, Avignon (France).
- "Flexibility, Defects & Disorder in Soft Porous Crystals", *Switchability in Porous Metal-Organic Frameworks*, 13-14 March 2017, Dresden (Germany).
- "Coupling transport and adsorption through Lattice Boltzmann methods", *EMN Meeting on Mesoporous Materials*, 13–17 June 2016, Prague (Czech Republic).
- "Mechanical impact of adsorption in compliant microporous materials", *12th International Conference on the Fundamentals of Adsorption*, 30 May to 3 June 2016, Friedrichshafen (Germany).
- "First-principles dynamics and free energy methods for flexible materials", *CP2K-UK Conference*, 22 February 2016, London (UK).
- "Computational characterization of flexibility and disorder: from the unit cell to the crystal", *Frontiers in Materials Science, Cambridge-JNCASR Winter School*, 7–11 December 2015, Bangalore (India).
- "Molecular simulation of materials flexibility and disorder", *International workshop on Flexibility and Disorder in Metal–Organic Frameworks*, 3–5 June 2015, Paris (France).
- "Polymorphism and Flexibility in Nanoporous Molecular Frameworks", *CPM-7: 7th International Workshop on the Characterization of Porous Materials*, 3–6 May 2015, Delray Beach FL (USA).
- "On the Impact of Adsorption in Compliant Nanoporous Materials", *4th Symposium on Future Challenges for Carbon-based Nanoporous Materials*, 16–18 March 2015, Nagano (Japan).
- "Interfaces and porous materials: Insight from Molecular Simulation", *CAPZEO-2014: Fourth International Summer School on Quantum Electronic Calculations*, 8–12 June 2014, Rabat (Morroco).
- "Theoretical Insight into Soft Porous Crystals", *CFCAM meeting on simulation of systems under thermodynamic gradients*, 25–26 March 2014, Paris (France).
- "Anisotropic Elastic Properties of Flexible Metal–Organic Frameworks", *International symposium on CO_2 capture*, 18–20 September 2013, Marne-la-Vallée (France).
- "Modeling of Soft Porous Crystals: From the Unit Cell to the Crystal", Gordon Research Conference *Nanoporous Materials & Their Applications*, 11–16 August 2013, Holderness NH (USA).
- "Structural transitions in metal–organic frameworks: thermodynamics & mechanics", *International workshop on adsorption in compliant solids*, 5–7 June 2013, Paris (France).
- "Ab Initio Investigation into the Hydration Mechanism of IRMOFs", CECAM/GDRi workshop on *Aging of Engineering Materials*, 8–10 February 2012, Zürich (Switzerland).
- "Effect of confinement on water in zeolite nanopores", *Indo French Seminar on Diffusion in Nanoporous and Dense Media*, 1–5 April 2009, Bangalore (India).
- "Water nanodroplets confined in zeolite pores", Faraday Discussion 141: *Water, From Interfaces to Bulk*, 27–29 August 2008, Edinburgh (UK).

In international conferences (27)

- "From crystal structure to properties: accelerating discovery of novel materials", *Fourth AiChemist School*, 4–11 March 2026, Paris (France).
- "Combining molecular simulation and machine learning to accelerate the discovery of materials with outstanding properties", *15th International Conference on the Fundamentals of Adsorption (FOA 15)*, 18–23 May 2025, Porto (Portugal).
- "Computational tools to discover novel materials and understand them", CECAM workshop on *Machine Learning Interatomic Potentials and Accessible Databases*, 9–11 September 2024, Grenoble (France).
- "Data-based understanding of supramolecular materials and their interactions with guest molecules", CECAM workshop on *Modelling Supramolecular Catalysis: Methods and Applications*, 12–14 May 2024, Paris (France).

- "Systematic exploration of framework materials properties: combining multi-scale modelling and machine learning", *MOF 2022 (8th International Conference on Metal-Organic Frameworks and Open Framework Compounds)*, 4–7 September 2022, Dresden (Germany)
- "Systematic exploration of nanoporous materials properties", *14th International Conference on the Fundamentals of Adsorption*, 22–27 May 2022, Denver CO (USA).
- "Systematic exploration of physical properties of nanoporous materials properties: combining quantum calculations, classical simulations, and machine learning", *FEZA 2021*, 5–9 July 2021, online.
- "Flexibility, Defects & Disorder in Soft Porous Crystals: Molecular Insight from Computational Chemistry", *12th International Conference on the Fundamentals of Adsorption*, 30 May – 3 June 2016, Friedrichshafen (Germany).
- "Assessing and predicting flexibility in MOFs with molecular simulation", *EUROMOF 2015, 1st European Conference on Metal Organic Frameworks and Porous Polymers*, 11–14 October 2015, Potsdam (Germany).
- "Molecular simulation of stimuli-responsive framework materials", *12th International Conference on Materials Chemistry (MC12)*, 20–23 July 2015, York (UK).
- "Polymorphism in nanoporous materials: assessing mechanical, thermal stability, and experimental feasibility", *249th ACS National Meeting* (PHYS division), 22–26 March 2015, Denver CO (USA).
- "Assessing and predicting flexibility in framework materials with molecular simulation", *249th ACS National Meeting* (COMP division), 22–26 March 2015, Denver CO (USA).
- "Remarkable Pressure Responses of MOFs: Proton Transfer, Linker Coiling, Order-to-Disorder Transitions", *249th ACS National Meeting* (PMSE division), 22–26 March 2015, Denver CO (USA).
- "Fluids in Soft Porous Crystals: Coupling Adsorption and Deformation", *RSC/IOP Joint Meeting on Computer Simulation of Confined Fluids*, 8 December 2014, London (UK).
- "Assessing and predicting flexibility in MOFs with molecular simulation", *IUCr 2014 — 23rd Congress and general assembly*, 5–12 August 2014, Montreal (Canada).
- "Mechanical Stability of Metal-Organic Frameworks: Insight from Molecular Simulation", *CONCREEP-9@MIT*, 22–25 September 2013, Cambridge MA (USA).
- "Anisotropic Elastic Properties of Flexible Metal–Organic Frameworks", *EUROMAT 2013*, 8–13 September 2013, Sevilla (France).
- "Understanding Stimuli-Induced Structural Transitions in MOFs", *17th International Zeolite Conference*, 7–12 July 2013, Moscow (Russia).
- "Ab Initio Investigation into the Hydration Mechanism of IRMOFs", *FOA11: 11th International Conference on the Fundamentals of Adsorption*, 19–24 May 2013, Baltimore MD (USA).
- "Ab Initio Investigation into the Hydration Mechanism of MOFs", *Characterization of Porous Media 6*, 30 April – 2 May 2012, Delray Beach FL (USA).
- "Water in Metal–Organic Frameworks", *Transient Chemical Structures in Dense Media*, 30 November 2010, Paris (France).
- "Thermodynamics of Guest-Induced Structural Transitions in Hybrid Organic–Inorganic Frameworks", International Zeolite Conference 16, 5–9 July 2010, Sorrento (Italy).
- "Adsorption of Water in Metal–Organic Frameworks: Insight From Molecular Simulation", *Fundamentals of Adsorption 10*, 24–30 May 2010, Awaji (Japan).
- "Water Intrusion in Hydrophobic Zeolites", *Fundamentals of Adsorption 10*, 24–30 May 2010, Awaji (Japan).
- "Effect of confinement on water in zeolite nanopores", XVIII International Conference on *Horizons in Hydrogen Bond Research*, 14–18 September 2009, Paris (France).
- "Water confined in nanopores : structure, dipole, IR and more", CECAM workshop on *New developments for first principles molecular dynamics simulations in condensed matter and molecular physics*, 15–18 May 2006, Lyon (France).
- "Elemental Femtochemistry of a Confined Hydrated Electron", Workshop on *Ab initio dynamical simulations in condensed matter*, 19 April 2006, Paris (France).

In national conferences (22)

- "Chimie théorique et méthodes basées sur les données en chimie", *Séance de prospective à l'Académie des Sciences*, 10 February 2026, Paris (France).

- "Méthodes basées sur les données en chimie : Accélérer le développement des matériaux", *Conférence « L'IA à Paris. Un an après le sommet, construire l'avenir »*, 9 February 2026, Paris (France).
- "Méthodes théoriques basées sur les données pour l'adsorption", *École de l'Association Française de l'Adsorption*, 26–28 January 2026, Anglet (France).
- "Concepts d'IA et Machine Learning et leur utilisation en chimie", *Colloque Chimie et Intelligence Artificielle*, 8 February 2023, Paris (France).
- "Discovery of Frameworks Materials with Targeted Properties by Machine Learning", *Méthodes Machine-Learning pour la Modélisation des Matériaux*, 22–24 September 2021, Toulouse (France).
- "Crystals with extraordinary behavior under stimulation", *GECOM CONCOORD*, 19–24 May 2019, Erquy (France).
- "Computational Chemistry of MOFs", *First French Congress on MOFs, COFs and Porous Polymers*, 16–17 May 2018, Paris (France).
- "Évolution de la communication scientifique", *Innométriques 2017*, 30 November 2017, Paris (France).
- "Dynamique moléculaire et méthode de Monte–Carlo", *DynaMol summer school*, 23–27 May 2016, Paris (France).
- "Matériaux intelligents et réactifs : comprendre et prédire leur comportement", *Journées francophones des jeunes physico-chimistes*, 19–23 October 2015, Girona (Spain).
- "Introduction to Molecular Dynamics and Monte Carlo simulations", *MeMoSim2015: Méthodes De Modélisation Et Simulation Multiéchelles*, 30 March – 2 April 2015, Lyon (France).
- "Des cristaux… mous et troués, mais intelligents !", *Journée Cristallographie à Chimie ParisTech* (dans le cadre de l'Année Internationale de la Cristallographie), 11 December 2014, Paris (France).
- "Theoretical insight into Soft Porous Crystals: Problems and tools to solve them", *Journées francophones des jeunes physico-chimistes*, 13–17 October 2014, Dammarie-les-Lys (France).
- "Anisotropic Elastic Properties of Flexible Metal-Organic Frameworks", Colloque Société Française de Physique, division *Physique Atomique, Moléculaire et Optique*, *Journées de Spectroscopie Moléculaire*, 7–10 July 2014, Reims (France).
- "Structure des Phases Adsorbées : Apports de la Simulation Moléculaire", *Journées École de l'Association Française de l'Adsorption*, 10 February 2014, Paris (France).
- "Ab Initio Investigation into the Hydration Mechanism of MOFs", *Journées 2013 de l'Association Française de l'Adsorption*, 14–15 February 2013, Paris (France).
- "Ab Initio Investigation into Hydrothermal Stability and Mechanical Properties of Soft Porous Crystals", *Atelier Simulation des Matériaux Désordonnés*, 12–13 December 2012, Marseille (France).
- "Adsorption & effets de confinement: Outils théoriques, simulation moléculaire", *GdR Thermodynamique Moléculaire et des Procédés*, 11 December 2012, Paris (France).
- "Modèles thermodynamiques et mécaniques pour la description des matériaux poreux flexibles", *Journées 2012 de l'Association Française de l'Adsorption*, 24–25 May 2012, Paris (France).
- "Adsorption & effets de confinement — Outils théoriques et simulation moléculaire", *Groupe Français d'Adsorption et des Surfaces Hétérogènes*, 2 July 2010, Paris (France).
- "Isothermes de type V de H2O et CO2 dans les MOF", *Groupe Français des Zéolithes*, 31 March – 2 May 2010, Giens (France).
- "Adsorption dans les matériaux nanoporeux flexibles", *Journées Modélisation à Paris*, 15–16 June 2009, Paris (France).

Invited seminars in research groups (28)

- Federal University of Rio de Janeiro (UFRJ) — ATOMS lab, 25 June 2026, online.
- École normale supérieure — PSL University, 3 April 2026, Paris (France).
- Université de Haute Alsace, 24 February 2026, Mulhouse (France).
- Saint-Gobain Recherche, 3 February 2021, Paris (France).
- University of Cambridge, 5 May 2020, online.
- University of Kyoto, 22 October 2019, Kyoto (Japan).
- Université Paris Diderot, 27 September 2019, Paris (France).
- Ruhr-Universität Bochum, 23 September 2019, Bochum (Germany).

- *Nature* publishing group, 8 July 2019, London (UK).
- Ruhr-Universität Bochum, 26 April 2018, Bochum (Germany).
- Ghent University, 25 April 2018, Ghent (Belgium).
- Université de Rennes, 16 February 2018, Rennes (France).
- Université de Haute Alsace, 16 October 2017, Mulhouse (France).
- iCeMS, University of Kyoto, 18 April 2017, Kyoto (Japan).
- Air Liquide, Delaware Research And Technology Center, 9 March 2017, Newark DE (USA).
- Université de Strasbourg, 11 October 2016, Strasbourg (France).
- Université Grenoble Alpes, 9 May 2016, Grenoble (France).
- Ghent University, 6 October 2015, Ghent (Belgium).
- Technische Universität Dresden, 8 July 2015, Dresden (Germany).
- Saint-Gobain/CNRS research lab, 18 March 2015, Cavaillon (France).
- École Normale Supérieure, 14 October 2014, Paris (France).
- University of Bath, 28 July 2014, Bath (UK).
- University of Oxford, 25 June 2014, Oxford (UK).
- Université de Bourgogne, 10 March 2014, Dijon (France).
- ENSICAEN / Université de Caen, 3 February 2014, Caen (France).
- Université de Strasbourg, 20 June 2013, Strasbourg (France).
- Université Paris Est, 18 January 2013, Paris (France).
- Universités d'Aix-Marseille, 15 June 2010, Marseille (France).

Community involvement

Editorial responsibilities

- Senior Editor for *Langmuir* (since 2026)
- Member of the International Commission on Metal–Organic Frameworks / IZA (since 2024)
- Scientific advisory board, ChemRxiv (since 2018)
- Editorial Advisory Board, *C&EN (Chemical and Engineering News)*, American Chemical Society (since 2016)
- Editorial Advisory Board, *Accounts of Materials Research* (since 2020)
- Editorial Board member for *Adsorption Science & Technology* (since 2019), former Associate Editor (2016–2019)
- Editorial Board member (External Editor) for *Communications Chemistry* (2018–2026)
- 2014–2019: Scientific Advisory Board for Chemistry at CNRS

Guest editor of journal special issues

- Collection on "Modelling and advanced characterization of framework materials" in *Communications Chemistry* (December 2023).
- Special issue on "Simulation of framework materials" in *Molecular Simulation* (Spring 2015).
- Special issue on "Flexibility and Disorder in Metal–Organic Frameworks" in *Dalton Transactions* (Early 2016).

Organization of conferences, workshops and tutorials

- Co-organizer of the International CECAM Workshop on "Modelling Supramolecular Catalysis: Methods and Applications", 12–14 May 2024, Paris (France).
- October 2020: co-chair of the Faraday Discussion on "Cooperative phenomena in framework materials" (planned in Sapporo, Japan; held online).
- Since May 2009: co-organizer of the meeting "Molecular modelling in Paris", a two-day national conference every Spring.

- Co-organizer of the International CECAM Workshop on Multi-scale modelling of flexible and disordered porous materials, 11–13 June 2018, Paris (France).
- Co-organizer of the International Workshop on "Flexibility and Disorder in Metal–Organic Frameworks", 3–5 June 2015, Paris (France).
- Co-organizer of the International Symposium on CO_2 capture, 18–20 September 2013, Marne-la-Vallée (France).
- Co-organizer of the International Workshop on "Adsorption in Compliant Solids", 5–7 June 2013, Paris (France).
- Co-organizer of the International Workshop on "Adsorption in Compliant Solids: Theory, Simulation, and Experiments", 9–11 June 2011, Paris (France).
- Co-organizer of a one-week tutorial on "Ab initio molecular dynamics with CPMD & CP2K", 6–9 April 2010, Paris (France).
- Organizing practicals at the "Quantum Simulation of Liquids and Solids" CECAM tutorial, 2006.

Peer-review and proposal review

- Reviewer of project proposals for the NSF and the French ANR (Agence Nationale de la Recherche).
- Reviewer for many journals, including: *Nature*, *Science*, *Nature Chemistry*, *Nature Materials*, *Phys. Rev. Lett.*, *J. Am. Chem. Soc.*, *Angewandte Chemie*, *Chem. Rev.*, *Chem. Soc. Rev.*, *Acc. Chem. Rev.*, *J. Phys. Chem.* (and *J. Phys. Chem. Lett.*), *PCCP*, *J. Mater. Chem.*, *Langmuir*, *Adsorption*, *Mol. Simulat.*, etc.

PhD students supervised (20)

- Yuanmei Yang, advisor: 2026–2029.
- William Xu, advisor: 2026–2029.
- Márcio Miguel da Silva Soares, co-advisor, University of Aveiro (Portugal): 2026–2029.
- Martin Bliek, advisor: 2025–2028. "Active learning to accelerate discovery of multi-variate MOFs"
- Fengming Shi, advisor: 2024–2027. "Studying amorphous solids and liquids through machine-learned potentials based on ab initio data"
- Léna Triestram, advisor: 2024–2027. "Accelerating the modeling of amorphous MOFs"
- Dune André, advisor: 2022–2025. "Modélisation de la structure et des propriétés de nouveaux matériaux amorphes"
- Lionel Zoubritzky, advisor: 2021–2024. "Methodology developments for the simulation of simple gas adsorption in nanoporous materials"
- Emmanuel Ren, advisor: 2020–2023. "Screening of the microscopic origins of Xe/Kr separation in nanoporous materials"
- Nicolas Castel, advisor: 2020–2023. "Atomistic models and properties of amorphous metal-organic frameworks for CO_2 separation"
- Maxime Ducamp, advisor, 2019–2022. "Materials with targeted responsive behaviour"
- Wenke Li, advisor, 2018–2021. "Computational simulation of CdSe quantum dots doped glasses"
- Guillaume Fraux, advisor: 2015–2019. "Molecular simulation of fluid adsorption in flexible nanoporous materials at multiple scales"
- Romain Gaillac, advisor, 2015–2018. "Molecular modelling of physics-chemical properties in microporous solids"
- Elsa Perrin, co-advisor (50%), 2015–2018. "Investigating silica nanoparticles / polymer composites: a coarse-grained molecular dynamics study"
- Liam Wilbraham, co-advisor (50%), 2014–2017. "Theoretical study of excited-state processes in the condensed phase"
- Jean-Mathieu Vanson, co-advisor (60%), 2014–2017. Interdépendence entre géométrie, adsorption et transport dans les matériaux à porosité hiérachique
- Aurélie Ortiz, co-advisor (80%), 2011–2014. "Étude par simulation moléculaire de la flexibilité des matériaux nanoporeux : propriétés structurales, mécaniques et thermodynamiques"
- David Bousquet, co-advisor (50%), 2010–2014. "Modélisation de l'adsorption dans les matériaux nanoporeux flexibles"
- Marta De Toni, co-advisor (80%), 2009–2012. "Simulation moléculaire de l'interaction de molécules polaires avec des matériaux de la famille des MOFs"

Post-doctoral researchers supervised (16)

- Arthur Hardiagon, 2023–2025.
- Luca Brugnoli, 2022–2024.
- Ambroise De Izarra, 2021–2023.
- Clément Wespiser, 2021.
- Thibaud Dreher, 2019–2020.
- Félix Mouhat, 2018–2020.
- Siwar Chibani, 2018–2020.
- Antoine Carof, 2018–2019.
- Jack Evans, 2015–2017.
- Clarisse Péan, 2015–2017.
- Fabien Trousselet, 2014–2016.
- Dario Corradini, 2014–2015.

- Quang-Tri Doan, 2012–2013.
- Jorge Peixinho, 2010–2011.
- Carlos Triguero, 2010–2012.
- Selvarengan Paranthaman, 2009–2010.

Habilitation (HDR) committees

- Vincent Dahirel (Sorbonne Université), December 2020.

PhD thesis committees (25)

- Moulay-Badr Attaiaa (supervisors: Matthieu Micoulaut & Stefan Klotz), June 2026. "Structure et dynamique de l'oxygène solide et des alliages O_2–N_2"
- Maria Chiara Notarangelo (supervisors: Emeric Bourasseau & Mathieu Salanne), April 2026. "Étude à l'échelle atomique des sels fondus à base d'américium — Application au calcul de propriétés thermophysiques"
- Sonia Salomoni (supervisors: Marco Saitta, Frédéric Datchi & Arthur France-Lanord), January 2026. "Machine Learning modeling approaches for polymorphism in liquid sulfur"
- Francesc Penas-Hidalgo (supervisors: Caroline Mellot-Draznieks & Albert Solé-Daura), October 2025. "Mechanistic Insights into CO_2 Valorization via Frustrated Lewis Pairs, Porphyrins, and Polyoxometalates: A Computational Approach"
- Virginia Guiotto (supervisors: Valentina Crocellà & Matteo Signorile), March 2025. "Exploring Metal-Organic Frameworks for the development of innovative composites: a new frontier for CO_2 separation"
- Srinidhi Mula (supervisor: Monique van der Veen), March 2024. "MOFs in Motion: Piezoelectricity and Rotational Dynamics of linkers in Metal–Organic Frameworks"
- Irene Bechis (supervisor: Kim Jelfs), May 2023. "Computational modelling of amorphous microporous materials"
- Mathilde Renouard (supervisor: Christian Serre), March 2023. "Vers de nouveaux matériaux poreux pour la capture d'odeurs de l'air habitacle"
- Maxime Langevin (supervisors: Rodolphe Vuilleumier & Marc Bianciotto), November 2022. "Generating drug-like molecules with artifical intelligence"
- Qing Wang (supervisors: Didier Tichit & Hazar Guesmi), October 2021. "Multi-Scale Theoretical Modeling of Pt- and Au-Based Catalysts Under Reactive Media"
- Benjamin Helfrecht (supervisor: Michele Ceriotti), June 2021. "Structure–Property Relationships in Complex Materials by Combining Supervised and Unsupervised Machine Learning"
- Adrian Gonzalez Nelson (supervisor: Freek Kapteijn & Monique A. van der Veen), May 2021. "Emergent rotational dynamics and optical properties of metal-organic frameworks"
- Valentin Gérard (supervisor: Élisabeth Charlaix), November 2020. "Technique d'intrusiométrie rapide pour l'étude du mouillage dynamique et du transport de soluté dans des pores hydrophobes nanométriques"
- Cyrille Takoukam Takoundjou (supervisor: Emeric Bourasseau), October 2020. "Étude du diagramme de phases du combustible MOX par simulation moléculaire de type Monte Carlo"
- Tung Doan (supervisor: Quy-Dong To), February 2020. "Homogenization of 2D nanoporous materials by combining micromechanics and molecular dynamics approaches"
- Boushra Mortada (supervisor: Claire Marichal), November 2019. "Synthesis of metal-organic frameworks for energetic applications"
- Johannes P. Dürholt (supervisor: Rochus Schmid), September 2019. "Force Field based Multiscale Simulations of Metal-Organic Frameworks"
- Sven Rogge (supervisor: Veronique Van Speybroeck), May 2018. "Derivation and Application of a Reliable Procedure to Computationally Model the Mechanical Stability of Rigid and Flexible Metal–Organic Frameworks"
- Laura Ronchi (supervisor: Jean Daou), October 2017. "Synthesis of hydrophobic zeolites for energetic applications"

- Henri Hay (supervisor: Guillaume Ferlat), September 2016. "Étude de la structure et des propriétés des polymorphes de SiO_2 et B_2O_3 par méthodes ab initio"
- Louis Vanduyfhuys (supervisor: Veronique Van Speybroeck), September 2015. "Insights in the Behaviour of Metal-Organic Frameworks through Molecular Modeling: from Force Field Derivation to Thermodynamic Analysis"
- François Villemot (supervisor: Benoit Coasne), November 2014. "Adsorption et transport dans des solides poreux hiérarchisés"
- Ines Collings (supervisor: Andrew Goodwin), June 2014. "Structure-property relationships in framework materials: anomalous mechanics by design"
- Benoît Carrier (supervisor: Henri Van Damme), December 2013. "Effet de l'eau sur les propriétés mécaniques à court et long termes des argiles gonflantes : expériences sur films autoporteurs et simulations moléculaires"
- Nicolas Ferrando (supervisor: Anne Boutin), June 2011. "Potentiels intermoléculaires et algorithmes de Monte Carlo : application à l'étude des composés oxygénés"