Paul Iacomi

Ph.D, M.Eng, 29 years old

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SUMMARY

Researcher specialised in the advanced characterisation of porous solids, I combine experimental and computational techniques to process, automate and obtain physical insights. Specifically, my research interests are the (i) synthesis (ii) characterisation and (iii) potential applications of novel porous materials, particularly in the fields of gas adsorption, gas separation, mechanical energy storage, and contaminant detection and capture. I have authored 15 publications in journals such as Nature Commun., JACS, Angewandte Chem., Chemical Science, Chemistry of Materials, etc. (10 as first author, 4 as corresponding author), which have been cited 208 times (h-index 8).

Keywords: porous coordination polymers, structure-property relationship, gas sorption and separation, thermomechanical energy storage, gas and vapour sensors, high pressure X-ray diffraction, characterisation of crystal defects, calorimetry and thermal methods.

RESEARCH INTERESTS

My main topic of research concerns the **characterisation and applications of novel porous framework materials**, such as metal-organic frameworks (MOFs), covalent-organic frameworks (COFs), coordination polymers (CPs) and composites thereof. This record-breaking and often counterintuitive class of materials have potential as tunable platforms for classical applications in gas sensing, capture, storage and separation or as highly selective catalysts. Moreover, they recently found innovative uses as molecular machines, energy converters or storage media.

My work can be divided into two main avenues. First is the **understanding of the nature of these materials at a fundamental level**. In this area, my research has explored the soft nature of hybrid porous networks, which allows them to undergo reconfigurable shifts in their structures in response to external stimuli. Their stimuli responsivity gives rise to novel behaviours such as "negative gas adsorption", which I have investigated from a thermodynamic point of view. Besides their soft nature, another prototypical feature of CPs is networks defects, with their characterisation and their influence on sorption properties a focus of my Marie Curie PhD.

The second research avenue concerns the **practical applications of porous hybrid materials**, in particular of their aforementioned compliant nature. Here, I have explored mechanical energy storage in frameworks which can act as nanosprings under fluid pressure. In a similar vein, I've explored the use of combined stimuli for exerting control over adsorption behaviour, such as by the use of external strain to control the uptake of CO_2. Other applications envisaged involve use of CPs as sensors, integrating them in electromechanical and electrochemical sensors to detect trace levels of contaminants such as volatile organic compounds.

Finally, throughout my research career I have also independently developed **tools for data mining, processing and aggregation pertaining to adsorption**, and applied them with the end goal of discovery and optimisation of materials for gas capture, storage, and separation. These standardised tools have been published as open-source software, serving as platform independent, transparent, and well-documented implementations of common processing techniques.

HIGHLIGHTED RESEARCH

Amongst my scientific output, three main research accomplishments are highlighted:

1. **Discovery and characterisation of the first known nanospring MOF for fully reversible storage.** A MOF dubbed CUK-1 was found to act as a molecular spring, switching under pressure with a change in volume of ~25%. Unlike all previously known materials, the switching pressure is identical for both compression and decompression, allowing stored work energy to be fully recovered. I further investigated this behaviour using *in-situ* high-pressure X-ray single crystal diffraction in collaboration with molecular modelling experts, yielding insight into the physical nature of the phenomenon (*Chemical Science*, **2021**, 12, 15, 5682–5687).

2. **Development of a data mining technique to discover and display interesting sorbent materials.** I instituted a data processing pipeline that would scrape publicly available adsorption data (totalling 30,000 adsorption isotherms) and calculate key performance indicators applicable to binary separations with the aim of ranking existing adsorbents and identifying overlooked materials. This project led to the publication of the resulting insights and interactive dashboard (*Chemistry of Materials*, **2020**, 32, 3, 982–991) as well as of the underlying adsorption processing codebase (*Adsorption*, **2019**, 25, 1533–1542). A related screening methodology was recently used to find a record-breaking material for siloxane vapour capture from biogas (*Journal of Materials Chemistry A*, **2021**, 9, 21, 12711–12720).

3. **Application of a challenging experimental technique to novel materials.** One of the major outcomes of my PhD consists in the application of low-temperature sorption microcalorimetry, a method developed in the MADIREL Lab, for the investigation of guest-host interactions in flexible MOFs of the type DUT-49. A Tian-Calvet immersion calorimeter device was specifically modified to operate at both 77 K and 87 K, alongside establishing non-trivial data processing methodologies. The use of four gas probes (N_2, Ar, O_2 and CO) was instrumental in observing the specifics of negative gas adsorption and allowed enthalpic and entropic effects to be classified. This first-author collaborative study was published in *Chemistry of Materials*, **2020**, 32, 8, 3489–3498.

SKILLS

Expert	Porous material characterisation through gas adsorption (gravimetric, volumetric, gas mixtures); X-ray diffraction for structural analysis; thermal analysis through microcalorimetry, thermogravimetry and differential scanning calorimetry.
Experienced	Single crystal diffraction; high pressure characterisation techniques (diamond anvil cells); Prototypical MOF synthesis (e.g. ZIF-8, UiO-66); thin film deposition, quartz-crystal resonator sensors, general spectroscopic techniques such as mass spectroscopy, gas phase chromatography, magnetic resonance imaging, infrared spectroscopy, classical force-field simulation methods.
IT skills	**Advanced:** Python, C++, LaTeX, Visual Basic, Microsoft Office **Fluent:** Linux/UNIX systems, Virtualization, Webdesign (HTML, CSS, JavaScript), Matlab, image processing, CAD + additive manufacturing
Language	Romanian — mother tongue English — bilingual French — fluent/C1 Mandarin Chinese — beginner/HSK1

WORK EXPERIENCE

Postdoctoral Researcher 04.2020–present

ICGM, CNRS / Université de Montpellier, France

Team DAMP, PI: Sabine DEVAUTOUR / Guillaume MAURIN

- Development of sensing methodology for monitoring the deposition of hazardous contaminants inside satellites. Project financed by the French Space Agency, Centre national d'études spatiales (CNES).
- Worked at the interface between high throughput material screening and electronic sensor manufacture to detect and quantify volatile vapours at trace levels. The research avenue involved the deposition of thin MOF layers on quartz supports and electrodes, requiring development of characterisation apparatus, alongside optimization of dispersion and deposition of nanoparticle solutions.

Postdoctoral Researcher 04.2019–03.2020

ICGM, CNRS / Université de Montpellier, France

Team DAMP, PI: Pascal YOT / Guillaume MAURIN

- Evaluation of coupling between mechanical pressure and adsorption for a molecular-level control over the gas separation and storage properties of flexible porous materials. Financed by ANR project ANR-17-CE29-0003, acronym MeaCoPA.
- Acquired extensive experience of powder and single crystal X-ray diffraction techniques under extreme pressure. With a budget of 30 000 euro, developed a prototype compression-adsorption diamond anvil cell in collaboration with Almax-EasyLAB.
- Taught 2 courses (50 hours) of laboratory tutorials to technical college students (DUT Chimie).

Postdoctoral Researcher 01.2019–03.2019

Laboratoire MADIREL, CNRS / Aix-Marseille Université, France

Team EnAP, PI: Philip LLEWELLYN

- Project coupling experimental and theoretical expertise to further understand the counterintuitive "negative gas adsorption" phenomenon in soft metal-organic frameworks. Financed by joint French (ANR) – German (DGA) research initiative ANR-17-CE08-0048, acronym FUN.
- I further developed and extended low-temperature calorimetry, a methodology created at the MADIREL lab, to be used for the study of flexible materials of the type DUT-49.

PhD in Condensed Materials and Nanoscience 10.2015–10.2018

Laboratoire MADIREL, CNRS / Aix-Marseille Université, France

Team EnAP, PI: Philip LLEWELLYN

- Characterisation of porous coordination frameworks to understand the complex interactions between crystal defects and adsorption, with the aim of evaluating them for applications such as catalysis, or gas storage and separation. Financed by an European H2020 Marie Curie ITN grant 641887, acronym DEFNET.
- Became an expert in adsorption techniques such as manometry, gravimetry, mixture adsorption, high pressure adsorption, columns and beds. Developed a complementary background in MOF synthesis, automation, thermal characterisation and spectroscopic characterisation of materials and interfaces (X-ray, IR, MRI).
- Together with other PhD students in DEFNET, organised *DocMOF 2018*, a symposium on Metal-Organic Frameworks with over 100 attendees from 70 institutions and 10 countries.

Internship, Engineering innovation 06-2013–09.2014

AkzoNobel ICI Paints, Slough, UK

Supply chain

- Involved in redesigning the quality control method for decorative paints for use in a lean, just-in-time manufacturing environment. Gained a strong background in automation, statistical analysis, colour science and rheology.
- Implemented a cleaning-in-place regime that succeeded in removing 99.993% of emulsion paint from a small-bore complex pipe system. The equipment helped reduce quality control time from 2–4 hours to 15 minutes.

PERSONAL PROJECTS

- Developed a Python codebase for standardised isotherm processing, released as an open source package (`https://github.com/pauliacomi/pyGAPS`).
- Visualisation dashboards that allow the processing and exploration of large datasets, such as discovering materials for binary gas separation (`https://pauliacomi.com/separation-explorer`) or music album rankings (`https://vortexplorer.herokuapp.com`).
- Created my website and blog (`https://pauliacomi.com`), and contributed to several open source projects (`https://github.com/pauliacomi`).

EDUCATION

PhD in Condensed Materials and Nanoscience 2015–2018
Aix-Marseille Université, France

- Thesis titled "Exploring Sources of Variability in Metal Organic Frameworks Through High Throughput Adsorption and Calorimetric Methods".

MEng (Hons) Chemical Engineering and Industrial Experience 2011–2015
University of Manchester, UK

- Four year integrated masters degree, with a year of experience in industry.
- Graduated with a 1st class degree. Received the Manchester Leadership Gold Award 2013.

ACADEMIC OUTPUT

Publications (in reverse chronological order)

[1] **P. Iacomi**, F. Alabarse, R. Appleyard, T. Lemaire, C. Thessieu, S. Wang, C. Serre, G. Maurin, P. G. Yot, "Structural Insight of MOFs under Combined Mechanical and Adsorption Stimuli", *Angewandte Chemie International Edition* **2022**, anie.202201924, DOI 10.1002/anie.202201924.

[2] **P. Iacomi**, G. Maurin, "ResponZIF Structures: Zeolitic Imidazolate Frameworks as Stimuli-Responsive Materials", *ACS Applied Materials & Interfaces* **2021**, acsami.1c12403, DOI 10.1021/acsami.1c12403.

[3] E. Amayuelas López, **P. Iacomi**, A. Fidalgo-Marijuan, B. Bazan, M.-K. Urtiaga, G. Barandika, L. Lezama, P. L. Llewellyn, M.-I. Arriortua, "Multifunctionality of Weak Ferromagnetic Porphyrin-Based MOF: Selective Adsorption in Liquid and Gas Phase", *CrystEngComm* **2021**, -, DOI 10.1039/D1CE00046B.

[4] E. Gulcay, **P. Iacomi**, Y. Ko, J.-S. Chang, G. Rioland, S. Devautour-Vinot, G. Maurin, "Breaking the Upper Bound of Siloxane Uptake: Metal-Organic Frameworks as an Adsorbent Platform", *J. Mater. Chem. A* **2021**, -, DOI 10.1039/D1TA02275J.

[5] J. Marreiros, R. de Oliveira-Silva, **P. Iacomi**, P. L. Llewellyn, R. Ameloot, D. Sakellariou, "Benchtop *In Situ* Measurement of Full Adsorption Isotherms by NMR", *J. Am. Chem. Soc.* **2021**, *143*, 8249–8254, DOI 10.1021/jacs.1c03716.

[6] **P. Iacomi**, J. S. Lee, L. Vanduyfhuys, K. H. Cho, P. Fertey, J. Wieme, D. Granier, G. Maurin, V. Van Speybroeck, J.-S. Chang, P. G. Yot, "Crystals Springing into Action: Metal–Organic Framework CUK-1 as a Pressure-Driven Molecular Spring", *Chem. Sci.* **2021**, *12*, 5682–5687, DOI 10.1039/D1SC00205H.

[7] S. Krause, J. D. Evans, V. Bon, I. Senkovska, S. Ehrling, P. Iacomi, D. M. Többens, D. Wallacher, M. S. Weiss, B. Zheng, P. G. Yot, G. Maurin, P. L. Llewellyn, F.-X. Coudert, S. Kaskel, "Engineering Micromechanics of Soft Porous Crystals for Negative Gas Adsorption", *Chem. Sci.* **2020**, *11*, 9468–9479, DOI 10.1039/D0SC03727C.

[8] **P. Iacomi**, P. L. Llewellyn, "Data Mining for Binary Separation Materials in Published Adsorption Isotherms", *Chemistry of Materials* **2020**, *32*, 982–991, DOI 10.1021/acs.chemmater.9b03376.

[9] **P. Iacomi**, B. Zheng, S. Krause, S. Kaskel, G. Maurin, P. L. Llewellyn, "Low Temperature Calorimetry Coupled with Molecular Simulations for an In-Depth Characterization of the Guest-Dependent Compliant Behavior of MOFs", *Chemistry of Materials* **2020**, *32*, 3489–3498, DOI 10.1021/acs.chemmater.0c00417.

[10] S. Krause, J. D. Evans, V. Bon, I. Senkovska, **P. Iacomi**, F. Kolbe, S. Ehrling, E. Troschke, J. Getzschmann, D. M. Többens, A. Franz, D. Wallacher, P. G. Yot, G. Maurin, E. Brunner, P. L. Llewellyn, F.-X. Coudert, S. Kaskel, "Towards General Network Architecture Design Criteria for Negative Gas Adsorption Transitions in Ultraporous Frameworks", *Nature Communications* **2019**, *10*, 3632, DOI 10.1038/s41467-019-11565-3.

[11] J. Marreiros, L. Van Dommelen, R. de Oliveira-Silva, G. Fleury, **P. Iacomi**, T. Stassin, S. Furukawa, P. Llewellyn, D. Sakellariou, M. Roeffaers, R. Ameloot, "Vapor-Phase Linker Exchange of the Metal-Organic Framework ZIF-8: A Solvent-Free Approach to Post-Synthetic Modification", *Angewandte Chemie International Edition* **2019**, *58*, 18471–18475, DOI 10.1002/anie.201912088.

[12] **P. Iacomi**, F. Formalik, J. Marreiros, J. Shang, J. Rogacka, A. Mohmeyer, P. Behrens, R. Ameloot, B. Kuchta, P. L. Llewellyn, "Role of Structural Defects in the Adsorption and Separation of C3 Hydrocarbons in Zr-Fumarate-MOF (MOF-801)", *Chemistry of Materials* **2019**, *31*, 8413–8423, DOI 10.1021/acs.chemmater.9b02322.

[13] **P. Iacomi**, U.-H. Lee, A. H. Valekar, J.-S. Chang, P. L. Llewellyn, "Investigating the Effect of Alumina Shaping on the Sorption Properties of Promising Metal–Organic Frameworks", *RSC Advances* **2019**, *9*, 7128–7135, DOI 10.1039/C9RA00534J.

[14] **P. Iacomi**, P. L. Llewellyn, "pyGAPS: A Python-Based Framework for Adsorption Isotherm Processing and Material Characterisation", *Adsorption* **2019**, *25*, 1533–1542, DOI 10.1007/s10450-019-00168-5.

[15] S. Krause, J. D. Evans, V. Bon, I. Senkovska, S. Ehrling, U. Stoeck, P. G. Yot, **P. Iacomi**, P. Llewellyn, G. Maurin, F.-X. Coudert, S. Kaskel, "Adsorption Contraction Mechanics: Understanding Breathing Energetics in Isoreticular Metal–Organic Frameworks", *The Journal of Physical Chemistry C* **2018**, *122*, 19171–19179, DOI 10.1021/acs.jpcc.8b04549.

Publications in press:

[1] **P. Iacomi**, E. Gulcay, G. Rioland, N. Stenou, S. Devautour-Vinot, G. Maurin, "Online sensor for volatile siloxanes integrating a mesoporous MOF", en, manuscript under review, **2022**.

[2] E. Gulcay, G. **P. Iacomi** Rioland, S. Devautour-Vinot, G. Maurin, "MOFs For Adsorption-Based Capture and Sensing of Toluene From Indoor Air: High-Throughput Screening To Experimental Validation", en, manuscript under preparation, **2022**.

Book chapters

[1] V. Bon, K. Roztocki, **P. Iacomi**, C. Hobday, I. Senkovska, A. Pöppl, E. Brunner, S. Kaskel in *The dynamic view: Multiscale Characterization Techniques for Flexible Frameworks*, (Ed.: S. Kitagawa), in press, RSC, **2022**.

Patents

[1] **P. Iacomi**, E. Gulcay, G. Rioland, S. Devautour-Vinot, G. Maurin (Centre National d'Études Spatiales, Centre National de la Recherche Scientifique, Université de Montpellier, Ecole Nationale Superieure de Chimie Montpellier), *French pat.*, FR2113602, **2021**.

Conference presentations (in reverse chronological order)

[1] **EuroMOF 2021**, Poland (virtual), October 2019; Oral presentation: *In situ XRD monitoring of compliant MOFs under combined mechanical and gas pressure*; **P. Iacomi**, F. Alabarse, G. Maurin, P. G. Yot

[2] **Frolic Goats Workshop 2021**, Poznań, Poland (virtual), March 2021; Oral presentation: *CUK-1 as the first reversible MOF molecular spring*; **P. Iacomi**, J. Wieme, J.-S. Chang, V. Van Speybroeck, G. Maurin, P. G. Yot.

[3] **Young EuroMOF Symposium 2019**, Paris, France, October 2019; Oral presentation: *Data mining for interesting separation materials in published adsorption isotherms*; **P. Iacomi**, P. L. Llewellyn

[4] **EuroMOF 2019**, Paris, France, October 2019; Oral presentation: *How external pressure provokes the structural switching of flexible MOFs?*; P. G. Yot, **P. Iacomi**, C. Serre, S. Kaskel, J.-S. Chang, V. Van Speybroeck, N. Stock, G. Maurin

[5] **MOF2018**, Auckland, New Zeeland, December 2018; Oral presentation: *Adsorption microcalorimetry at low temperatures for elucidating the compliant behaviour of DUT-49 and analogues*; **P. Iacomi**, S. Krause, S. Kaskel, P. L. Llewellyn

[6] **ESTAC12**, Brasov, Romania, August 2018; Oral presentation: *Using low temperature calorimetry for in situ monitoring of the switching behaviour of a flexible metal organic framework DUT-49*; **P. Iacomi**, S. Krause, S. Kaskel, P. L. Llewellyn

[7] **CPM-8**, Delray Beach, USA, May 2018; Poster presentation: *pyGAPS: A Python Adsorption Isotherm Processing Suite*; **P. Iacomi**, P. L. Llewellyn

[8] **MC2**, Zurich, Switzerland, January 2018; Oral presentation: *Using calorimetry to further understand the phenomenon of "Negative Gas Adsorption" in DUT-49 and its family of materials*; **P. Iacomi**, S. Krause, S. Kaskel, P. L. Llewellyn

[9] **EuroMOF**, Delft, Netherlands, November 2017; Poster presentation: *Insights obtained through bulk processing of isotherm and calorimetry data and their applications for adsorbent fingerprinting* ; **P. Iacomi**, A. D. Wiersum, N. Chanut, P. L. Llewellyn

[10] **MOF2016**, Long Beach, USA, September 2016; Poster presentation: *Effect of Shaping MOFs on Adsorption Performance Investigated Using Adsorption Microcalorimetry*; **P. Iacomi**, N. Chanut, A. D. Wiersum, U-H. Lee, Y. K. Hwang, F. Ragon, H. Chevreau, S. Bourrelly, B. Kuchta, J-S. Chang, C. Serre, P. L. Llewellyn