

Paul Iacomi

Ph.D, M.Eng, 28 years old

Contact: +33 (0) 7 68 46 61 19
mail@pauliacomi.com
www.pauliacomi.com

SUMMARY

Researcher with a background in chemical engineering and materials science. I combine experimental and computational techniques to process, automate and obtain physical insights. My academic output is related to the (i) synthesis (ii) characterisation and (iii) potential applications of novel metal-organic framework (MOF) porous materials.

HIGHLIGHTED RESEARCH

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

1. 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 personal 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).

2. 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 previously developed in the MADIREL Lab, for the investigation of guest-host interactions in flexible MOFs of the type DUT-49. The 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 (N₂, Ar, O₂ and CO) was instrumental in observing the highly differing 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.

PROFESSIONAL EXPERIENCE

Postdoctoral Researcher

04.2020–now

ICGM, CNRS / Université de Montpellier, France

Team DAMP, PI: Sabine DEVAUTOUR

- Development of sensing methodology for monitoring the deposition of hazardous contaminants inside satellites. Project financed by the 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.

Postdoctoral Researcher

04.2019–03.2020

ICGM, CNRS / Université de Montpellier, France

Team DAMP, PI: Pascal YOT

- 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

- Research topic focused on characterisation 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, molecular modelling and spectroscopic characterisation of materials and interfaces (X-ray, infrared, 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.

FREELANCE 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.

SKILLS

<i>Expert</i>	Materials characterisation through gas adsorption (gravimetric, volumetric, gas mixtures); X-ray diffraction for structural analysis; thermal analysis through microcalorimetry, thermogravimetry and differential scanning calorimetry.
<i>Experienced</i>	Prototypical MOF synthesis (e.g. ZIF-8, UiO-66); single crystal diffraction; high pressure characterisation techniques (diamond anvil cells); other spectroscopic techniques such as mass spectroscopy, gas phase chromatography, magnetic resonance imaging, infrared spectroscopy.
<i>Languages</i>	Romanian (mother tongue) English (bilingual) French (fluent)
<i>IT skills</i>	Advanced: Python, C++, \LaTeX , Visual Basic, Microsoft Office Fluent: Linux/UNIX systems, Virtualization, Webdesign (HTML, CSS, JavaScript), Matlab, image processing, CAD + additive manufacturing

ACADEMIC OUTPUT

0.1 Publications (in reverse chronological order)

- [1] S. Krause, J. D. Evans, V. Bon, I. Senkovska, S. Ehrling, **P. Iacomi**, D. M. Többs, P. L. Llewellyn, D. Wallacher, M. S. Weiss, B. Zheng, P. G. Yot, G. Maurin, F.-X. Coudert, S. Kaskel, “Engineering Micromechanics of Soft Porous Crystals for Negative Gas Adsorption”, *Chemical Science* **2020**, 10.1039.D0SC03727C, DOI 10.1039/D0SC03727C.
- [2] **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.
- [3] **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.
- [4] S. Krause, J. D. Evans, V. Bon, I. Senkovska, **P. Iacomi**, F. Kolbe, S. Ehrling, E. Troschke, J. Getzschmann, D. M. Többs, 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.
- [5] J. Marreiros, L. Van Dommelen, R. de Oliveira-Silva, G. Fleury, **P. Iacomi**, T. Stassin, S. Furukawa, P. Llewellyn, D. Sakellariou, M. Roeflaers, 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.
- [6] **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.

- [7] **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.
- [8] **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.
- [9] 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 Isorecticular Metal–Organic Frameworks", *The Journal of Physical Chemistry C* **2018**, 122, 19171–19179, DOI 10.1021/acs.jpcc.8b04549.

Including work currently in preparation:

- [1] **P. Iacomi**, G. Maurin, "ResponZIF structures: zeolitic imidazolate frameworks as stimuli-responsive materials", en, review, manuscript in preparation, **2020**.
- [2] **P. Iacomi**, L. Vanduyfhuys, K. H. Cho, J. S. Lee, J. Wieme, P. Fertey, D. Granier, G. Maurin, J.-S. Chang, V. Van Speybroeck, P. G. Yot, "Springtime Under Pressure: Metal-Organic Framework CUK-1 as a Fully Reversible Molecular Spring", en, manuscript submitted to JACS, **2020**.
- [3] J. Marreiros, R. de Oliveira-Silva, **P. Iacomi**, P. Llewellyn, R. Ameloot, D. Sakellariou, "Simultaneous ultra-compact NMR and physisorption for full-isotherm adsorption characterisation", en, manuscript submitted to Nature Materials, **2020**.

0.2 Conference presentations

- [1] **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
- [2] **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
- [3] **MOF2018**, Auckland, New Zealand, 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
- [4] **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
- [5] **CPM-8**, Delray Beach, USA, May 2018; Poster presentation: *pyGAPS: A Python Adsorption Isotherm Processing Suite*; **P. Iacomi**, P. L. Llewellyn
- [6] **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
- [7] **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
- [8] **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