

Ciclo di incontri – Tavolo di discussione

CRYSTALLITE SIZE:

TAILORING INTRUSION-EXTRUSION SYSTEMS FOR APPLICATION

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The behaviour of Heterogeneous Lyophobic Systems (HLSs) comprised of a lyophobic porous material and a corresponding non-wetting liquid is affected by a variety of different structural parameters of the porous material. Dependence on an exogeneous property such as crystallite size is desirable for system tuning, as it is easily modified. We explore the dependence of intrusion/extrusion pressures and intruded volume on crystallite size, testing the hypothesis that the connection between internal cavities and bulk water facilitates intrusion via hydrogen bonding, a phenomenon that is magnified in smaller crystallites with a larger surface/volume ratio.¹

In addition, other properties are explored: flexibility, negative compressibility,² heat of intrusion/extrusion, ^{3,4} and finally contact electrification,⁵ a concept which is at the heart of the ElectroIntrusion project.

References

- (1) Johnson, L. J. W.; Paulo, G.; Bartolomé, L.; Amayuelas, E.; Gubbiotti, A.; Mirani, D.; Le Donne, A.; López, G. A.; Grancini, G.; Zajdel, P.; Meloni, S.; Giacomello, A.; Grosu, Y. Optimization of the Wetting-Drying Characteristics of Hydrophobic Metal Organic Frameworks via Crystallite Size: The Role of Hydrogen Bonding between Intruded and Bulk Liquid. *Journal of Colloid and Interface Science* 2023, 645, 775–783. <https://doi.org/10.1016/j.jcis.2023.04.059>.
- (2) Johnson, L. J. W.; Mirani, D.; Le Donne, A.; Bartolomé, L.; Amayuelas, E.; López, G. A.; Grancini, G.; Carter, M.; Yakovenko, A. A.; Trump, B. A.; Meloni, S.; Zajdel, P.; Grosu, Y. Effect of Crystallite Size on the Flexibility and Negative Compressibility of Hydrophobic Metal–Organic Frameworks. *Nano Lett.* 2023, 23 (23), 10682–10686. <https://doi.org/10.1021/acs.nanolett.3c02431>.
- (3) Lowe, A. R.; Ślęczkowski, P.; Arkan, E.; Le Donne, A.; Bartolomé, L.; Amayuelas, E.; Zajdel, P.; Chorążewski, M.; Meloni, S.; Grosu, Y. Exploring the Heat of Water Intrusion into a Metal–Organic Framework by Experiment and Simulation. *ACS Appl. Mater. Interfaces* 2024, 16 (4), 5286–5293. <https://doi.org/10.1021/acsami.3c15447>.
- (4) Johnson, L. J. W.; Lowe, A. R.; Le Donne, A.; Arkan, E.; Merchiori, S.; Bartolomé, L.; Amayuelas, E.; Mirani, D.; López, G. A.; Grancini, G.; Chorążewski, M.; Meloni, S.; Grosu, Y. Crystallite Size Effects on the Heat of Water Intrusion/Extrusion into/from Metal–Organic Frameworks. Under Review.
- (5) Bartolomé, L.; Littlefair, J. D.; Amayuelas, E.; Johnson, L. J. W.; Le Donne, A.; Šutka, A.; Meloni, S.; Grosu, Y. Triboelectrification During Water Intrusion–Extrusion into-from Hydrophobic Nanopores. *Advanced Materials Technologies* n/a (n/a), 2401744. <https://doi.org/10.1002/admt.202401744>.

Wednesday the 5th of February 2025 – 11.00 – Sala Videoconferenze

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