

## 2<sup>nd</sup> International Seminar on Modelling, Simulation and Machine Learning for the Rapid Development of Porous Materials - Workshop Program

### First Day, Tuesday, March 05, 2024

09:15	Maciej Haranczyk & Organizers	Introduction and Welcome
09:25	William Gonçalves (INSA Lyon)	Aerogel simulations based on molecular dynamics and tomography input, review and future trends
09:55	Fadi Aldakheel (Leibniz Universität Hannover)	Failure mechanisms of fluid saturated porous materials
10:25	Prakul Pandit (Institute of Materials Research - DLR)	Towards sustainable material development: Computational modelling of (Aero)-gels
11:00	<b>Coffee break with poster session*</b>	
11:30	Pavel Gurikov (Technische Universität Hamburg)	Insights into dynamics of primary fibers in nanofibrous porous materials with coarse-grained models
11:50	Nina Borzęcka (Institute of Materials Research -DLR)	Insights into modelling the gelation process in cellulose aerogels
12:10	Michał Bogdan (Polish Academy of Sciences)	Discreteness, stochasticity, geometry, topology and mechanical energy in small soft granular structures.
12:30	Zoltán Balogh (University of Debrecen)	Wetting of alginate aerogels, from mesoporous solids to hydrogels: a small-angle scattering analysis
12:50	<b>Lunch with poster session</b>	
14:00	Ameya Rege (Institute of Materials Research - DLR)	Molecular description of nanostructured porous materials
14:20	Kathrin Eckert (Technische Universität Hamburg)	Unveiling the thermodynamics of stimuli-responsive gels: A COSMO-RS and Molecular Dynamics study
14:40	Sergei Zorkaltsev (IMDEA Materials)	Predicting mechanical properties of topologically defined nanoporous metal structures with Machine Learning
15:00	Rajesh Chandrasekaran (RWTH Aachen University)	Correlation between structure and thermal conductivity of air-saturated open-porous materials
15:20	<b>Coffee break with poster session</b>	
15:50	Beatriz Merillas (University of Valladolid)	Challenges in modelling the thermal conductivity of super-insulating aerogels
16:10	Nabil Abomailek (IMDEA Materials)	Experimental and computational study of the formation of aerogels from aerosols of nanowires
16:30	Lucas Mager (Universität zu Köln)	Data-driven surrogate models for an efficient numerical homogenization of biopolymer aerogels
16:50	Rasul Abdusalamov (RWTH Aachen University)	Microstructural characterization in aerogel modeling through Deep Symbolic Regression
17:10	<b>Visit to the facilities of IMDEA Materials</b>	
18:00	<b>Bus to Atocha Station</b>	

\*Poster presenters: Carlos Illanes-Bordomás, Jimena de la Vega, Burcu Ozdemir, Miguel Hernández del Valle, Christina Schenk

Location:  
IMDEA Materials Institute,  
c/Eric Kandel 2, Getafe, Madrid

March 4-6, 2024

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### Second Day, Wednesday 06, 2024

09:15	Berend Smit (EPFL)	Exploring the Unseen: Big Data's Role in the Evolution of Nanoporous Material Studies
10:00	Susana Garcia (Heriot-Watt University)	From Data to Deployment: The Role of Stakeholder Perspectives in Advancing ML-enhanced materials design
10:30	German Sastre (UPV-CSIC)	Computational Design of New Organic Structure Directing Agents for the Synthesis of Zeolites Using Big Data
11:00	<b>Coffee break with poster session</b>	
11:30	Peyman Z. Moghadam (University College London)	The CSD MOF subset: High-throughput Computational Screening for Materials Discovery
12:00	Paweł Dłotko (Polish Academy of Sciences)	Topological methods in material analysis and design
12:30	Mariana Landin Pérez (University of Santiago de Compostela)	Reduced experimental designs and genetic algorithms for porous core-shell microparticles development
12:50	Alechania Misturini (ICMol, Universitat de València)	Effect of intracrystalline silanol defects on benzene diffusivity in silicalite
13:10	<b>Lunch with poster session</b>	
14:15	Marcus Noack (Berkeley Lab)	Gaussian Processes and High-Performance Mathematical Optimization for Optimal and Autonomous Data Acquisition
15:00	Cory Simon (Oregon State)	Multi-fidelity Bayesian optimization of covalent organic frameworks for xenon/krypton separations
15:30	<b>Coffee break with poster session</b>	
15:50	Phuong Vo (IMDEA Materials)	Exploring interface characteristics and thermal conductivity in MOF/Polymer Mixed Matrix Membrane Composites through atomistic simulations
16:10	Giulia Lo Dico (Tolsa SL)	Machine-learning-accelerated design of clay-based porous materials
16:30	Junchen Xiao (IMDEA Materials)	Predicting the of mechanical and flame-retardant properties of MOF-added polymer nanocomposites
16:50	Preethi Aranala Gurumoorthi (Technische Universität Hamburg)	Computer-Aided Solvent Design for Microgel Synthesis Processes
17:10	<b>Closing remarks</b>	
17:15	Informal discussions and software demos	
18:00	<b>Bus to Atocha Station**</b>	

\*\*alternative transport times can be organized if necessary (contact the Organizers to arrange)

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