



InterPore2025

Monday, 19 May 2025

MS24: 1.2 (13:50 - 15:05)

time	[id] title	presenter
13:50	[88] Molecular Modeling of the Structure and Dynamics of Nanoconfined Fluids	GREATHOUSE, Jeffery
14:05	[119] Adsorption-Induced Deformation and Its Impact on Gas Transport in Microporous Coal Matrix	Mr YANG, Quanlin
14:20	[28] Molecular Insights into Caprock Integrity of Subsurface Hydrogen Storage: Perspective on Hydrogen-induced Swelling and Mechanical Response	Mr GHASEMI, Mehdi
14:35	[356] Molecular Modeling of Structure, Diffusion, and Electrical Conductivity of Ionic Aqueous Solutions in Bulk and Confined within Nanoporous Media.	AMARO ESTRADA, Jorge Ivan
14:50	[401] Accelerating Type 3 Porous Liquid Discovery for Carbon Capture	Dr ROBINSON BROWN, Dennis

# Tuesday, 20 May 2025

## MS24: 2.1 (09:05 - 10:05)

time	[id] title	presenter
09:05	[29] Developing Effective Sorbents for Direct Air Capture using Large-scale DFT Calculations and ML Forcefields	SHOLL, David
09:20	[83] Machine-Learned Force Field Development for Molecular Simulation of CO <sub>2</sub> Adsorption/Desorption in UiO-66 Metal-Organic Frameworks	Mr JALALMANESH, Shayan
09:35	[24] Ab Initio Molecular Dynamics Investigation of Water and Butanone Adsorption on UiO-66 with Defects	CHOUDHURI, Deep
09:50	[376] Molecular dynamics study of swelling of wood-inspired polymeric composite and other interactions with water	Prof. DEROME, Dominique