EFCE Spotlight Talks

Section on Artificial Intelligence for Chemical Engineering (AI4CE)

3 November 2026

14:00-16:00 CET

EFCE

From Pore to Plant: AI Across the Adsorption Chain

Adsorption turns up almost everywhere in chemical engineering, carbon capture, water treatment, gas drying, biopharmaceutical purification, and it is one of the few operations where a choice made at the scale of a pore ends up deciding what the plant can do. That chain, from the pore to the process, has traditionally been split across communities that rarely talk to each other, and AI is now starting to close it. This webinar follows the chain end to end. The first talk deals with molecular simulation and machine learning for nanoporous materials, where it is possible to screen candidates before any of them exists in a laboratory. The second brings the discussion to the bench, on how AI supports experimental campaigns and turns adsorption measurements into data one can actually use. The third takes it to the process side, on model-based and data-driven design of chromatographic separations. The session is not addressed only to the adsorption community: if you work on separations, on materials, or on where AI earns its place in process engineering, it was put together with you in mind. The three speakers are women, and the line-up is the first activity of the Women in AI4CE initiative.

PROGRAM

14:00	**Welcome and introduction** Idelfonso B. R. Nogueira, Chair of the Section AI for Chem. Eng., NTNU – Norway Mattia Vallerio, co-chair of the Section AI for Chem. Eng., Politecnico di Milano - Italy Maria Papathanasiou, lead of Women in AI4CE initiative, Imperial College London - UK António Gonçalves da Silva, EFCE Executive Vice-President
14:10	**Designing the material before it exists: molecular simulation and machine learning for nanoporous adsorbents** Sofia Calero, Eindhoven University of Technology - the Netherlands
14:40	**AI in the adsorption laboratory: from the experimental campaign to data one can use** Nina Salau, UFSM - Brazil
15:10	**AI and model-based design of chromatographic separation processes** Maria Papathanasiou, Imperial College London - United Kingdom
15:40	**Round-table discussion with the three speakers and conclusion** Idelfonso B. R. Nogueira, Chair of the Section AI for Chem. Eng., NTNU – Norway Mattia Vallerio, co-chair of the Section AI for Chem. Eng., Politecnico di Milano - Italy

REGISTRATION

free of charge but mandatory

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