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CCP5 Workshop: Adsorption in Novel Porous Materials

Manchester, UK

Flor R. Siperstein

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A large variety of novel porous materials has emerged in the last decades, from metal organic frameworks to microporous polymers. The challenges associated with modelling these materials range from the availability of reliable force fields to the need of capturing phenomena that is not observed in conventional adsorbents, like swelling or slow relaxation processes. In this workshop we discussed current methods being used for modelling adsorption in novel porous materials, their applicability and limitations.

The meeting took place in room C53/64 in the Mill building at the University of Manchester and had approximately 30 participants. The structure of the meeting consisted on a number of invited and contributed presentations followed by a short discussion. The workshop programme was:

10.30-11:15 Registration

11.15-12:00 Carlos Nieto, IFP "Molecular simulation of Zeolitic Organic Frameworks"

12:00-13:00 Lunch

13:00-13.30 Tina Duren, U. Edinburgh "Using molecular simulation to characterise metal-organic frameworks"

13.30-14:00 Rochus Schmid, Ruhr-Universität Bochum "First principles derived force fields for structure and dynamics of porous coordination polymers"

14:00-14:30 Abbie Trewin, U. Liverpool "Microporous polymers"

14:30-15:00 Break

15:00-15:30 Lev Sarkisov, U. Edinburgh "Imprinted polymers"

15:30-15:50 Erich Muller, Imperial College London "Adsorption and permeation on microporous carbon and polymer membranes from non-equilibrium steady state molecular dynamics simulations"

15:50-16:10 Richard Henchman, U. Manchester "From Diffusion in Polymers to Water"

16:10-16:30 Paola Carbone, U. Manchester "An hybrid approach to study the diffusion of gas particles in amorphous structures"

More information is available in the workshop website: www.adsorptionworkshop.org

Budget

Travel & accommodation (speakers)	£687.95
Catering	296.19
Total	£984.14

Participants

	First name	Last Name	Affiliation	Email
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(invited speakers in bold)