(i)RASPA online school/workshop:
Software for visualization and simulation of porous materials and fluids

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January 11, 2021 (online)
Registration (free but compulsory) via: www.iraspa.org
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This workshop/school focuses on a practical understanding of visualization and molecular simulation of nanoporous materials and fluids, using iRASPA and RASPA. RASPA is well known for force field-based molecular simulation of adsorption and diffusion in nanoporous materials (such as MOFs and zeolites), as well as studying thermodynamic and transport properties of complex fluids. The combination with the visualization software iRASPA enables obtaining direct molecular insight. In this ½ day workshop, besides lectures on the basics of MD/MC, we will also consider the practical side of simulations using iRASPA/RASPA: setting up the system, constructing input files for molecules and frameworks, setting up a force field, understanding input settings, and analyzing the output. The workshop will be online.

Program January 11, 2021
(all times are CET, Central European Time)

13h00 – 13h10 Welcome and introduction (Prof. Sofia Calero)

13h10 – 14h00 Visualization of porous structures using iRASPA (Dr. David Dubbeldam)

14h00 – 14h30 Introduction to molecular simulation and force fields (Prof. Sofia Calero)

14h30 – 14h45 short break

14h45 – 15h15 Monte Carlo simulation in different ensembles (Prof. Thijs J.H. Vlugt)

15h15 – 15h45 Molecular Dynamics simulation (Prof. Randy Q. Snurr)

15h45 – 16h15 Computing adsorption isotherms in MOFs with RASPA (Dr. Juan José Gutierrez Sevillano)

16h15 – 16h30 short break

16h30 – 17h45 Questions & answers session with all lecturers