“Digital Adsorption Data Space”

A IUPAC Task Force Symposium

Registration link for participants:
https://attendee.gotowebinar.com/register/2859336492764167765

May 30th, 2023

11.30-15.40 CET

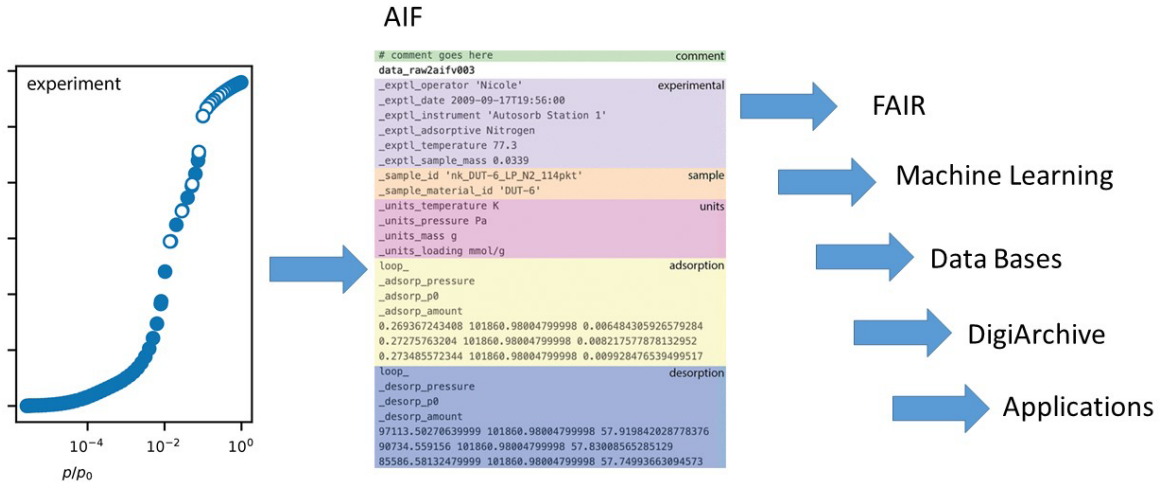
Time (CET)	Title	Speaker
11.30 – 11.50	Introduction and Scope	Stefan Kaskel, TU Dresden
11.50 -12.20	Adsorption Information File: Tools (How to convert experimental data)	Jack Evans, Univ. of Adelaide
12.20 -12.50	On the challenges of simulating accurate adsorption properties and their data management	Veronique van Speybroeck/ Louis Vanduyfhuys (Ghent University)
12.50 -13.20	Problematic Isotherm Data, Quiz	Dan Siderius (NIST)
13.20 -14.00	Discussion, Q&A	All
14.00-15.00	Contributed Short Presentations from Users: Applications	Porous Carbons (Joaquin Silvestre-Albero), MOFs: Seda Keskin (Koc University), Volodymyr Bon (TU Dresden), Data Visualization with pygaps: Paul Iacomi (SMS), High Pressure Data: Darren Broom (Hiden)
15.00-15.30	NIST Adsorption Database	Dan Siderius (NIST)
15.30-15.40	Closing remarks	Stefan Kaskel, TU Dresden

New advanced adsorbents are a crucial driver for the development of energy and environmental applications. There is tremendous potential provided by machine

learning and data mining techniques to identify an adsorbent for a particular application. However, the current scientific reporting of adsorption isotherms in graphs and figures is not adequate to reproduce original experimentally measured data.

In our interactive workshop, advanced data formats and their implementation in publications and databases are illustrated. Specifically, we present a new standard format for isotherms, the Adsorption Information File (AIF), which is built on the self-defining text archive and retrieval (STAR) format that is similarly used for the ubiquitous Crystallographic Information File. The AIF is a flexible, general and easily extended free-format archive file that is readily human and machine readable - simple to edit using a basic text editor or to parse for database curation.

Applications of adsorption data archiving, visualization and interaction with the NIST isotherm database for a wide range of porous materials (activated carbons, metal-organic frameworks, high pressure data etc.) will be discussed including experimental and simulation data (e.g. RASPA data).



Archiving adsorption data in an advanced, open, and consistent format following FAIR guidelines will facilitate the electronic transmission of adsorption data between laboratories, journals and larger databases and increase opportunities for open science in the field of adsorption by porous materials, nanomaterials and catalysts in future.