



Contribution ID: 12

Type: Oral Presentation

Dissemination and updates to the universal standard archive file for adsorption data

Tuesday, May 21, 2024 11:10 AM (20 minutes)

Porous materials have shown remarkable effectiveness in energy and environmental applications. However, the current method of presenting adsorption isotherms through graphs and figures falls short in terms of reproducibility, reuse, and data sharing. It is crucial to promote open science in the field of porous materials for future researchers [1].

Since 2021, we have developed a novel standard adsorption information file (AIF), taking inspiration from the widely used crystallographic information file (CIF) [2]. The AIF is a versatile and easily expandable archive file format that is both human and machine-readable. We are continuously enhancing the format to meet the requirements of researchers. This initiative marks the first steps toward an open adsorption data format, simplifying the exchange of adsorption data among laboratories, journals, databases, and the scientific community. The adoption of this format is gaining momentum, driven by the support of IUPAC (<https://iupac.org/project/2021-016-1-024/>).

The standardized reporting of adsorption isotherms will enable the application of advanced AI methods (machine learning etc.) to develop innovative processes for separation and environmental technologies and accelerate the finding of high performance porous materials for such operations.

Primary authors: Dr SIDERIUS, Daniel (NIST); Dr EVANS, Jack (Univ. Adelaide); KASKEL, Stefan (Fraunhofer IWS & TU Dresden)

Presenter: KASKEL, Stefan (Fraunhofer IWS & TU Dresden)

Session Classification: Tuesday

Track Classification: Oral Presentations