

Data Resources for Adsorption: Isotherms, Adsorbent Materials, Formatting Standards, and User Data Submission

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In 2014, the National Institute of Standards and Technology (NIST), in cooperation with the Advanced Research Projects Agency–Energy (ARPA-E) of the U.S. Department of Energy, released a web-based database for cataloging adsorption isotherms and adsorbent materials, the NIST/ARPA-E Database of Novel and Emerging Adsorbent Materials. Users can use this tool to obtain reference data for adsorbent materials and adsorption isotherms, for comparison with their own measurements, to test and calibrate equipment, or to screen adsorbents and adsorbates for desired behavior or properties. The data in this database, which are available through both a web-based application and an application programming interface (API) are obtained from open sources in the scientific literature and measurements at participating laboratories, including the NIST Facility for Adsorbent Characterization and Testing. In this work, we discuss the developments of this database since its initial release, including its extension to multicomponent adsorption systems, both to advertise newer features and foster broader usage by the broad community studying adsorbent materials. In particular, we discuss the development of a formatting standard for describing adsorption isotherms (the JSON isotherm format) that allows for unambiguous description of multicomponent adsorption data. Building on this isotherm formatting standard, we also discuss git-based workflows and digitization tools for contributing isotherm data corrections and new data, both of which are intended to improve the accuracy of the database contents and improve data fidelity. Finally, we discuss future directions for the database and possible features in a third iteration of the application and API.