The NIST/ARPA-E Database of Novel and Emerging Adsorbent Materials: An Online Infrastructure for Cataloging and Curating Adsorbent Materials, Data, and Properties

Daniel Siderius [C, S], Vincent Shen, Russell Johnson and Roger van Zee
Chemical Sciences Division, NIST, Gaithersburg, MD, U.S.A.
daniel.siderius@nist.gov

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, has developed a web-based database for cataloging adsorbent materials and curating data regarding adsorption of gases by those materials. This new Standard Reference Data product is intended to be used to disseminate data and properties of the cataloged adsorption systems for use by groups across disciplines and sectors, including industry, academia, instrument manufacturers, standards bodies, and government laboratories. Interested parties can access this tool for comparison with their own measurements, to test and calibrate equipment, or to screen adsorbents and adsorbates for desired behavior or properties. The data for adsorbent materials, adsorbate fluids, and their interactions 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 present the new database and web application to the gas adsorption community and discuss its goals, both to advertise the new resource and to foster conversations that will improve the goals and future direction of the work so that it is a truly beneficial to the broad community studying adsorbent materials and those utilizing porous materials for end applications. We also discuss pitfalls encountered while gathering adsorption data from the scientific literature related to inconsistencies and common errors in data presentation. These difficulties, however, have also identified opportunities for standardizing the presentation of adsorption data, which could greatly aid comparisons of adsorption data from different laboratories as well as ease the inclusion of newly-measured adsorption data into the NIST database. Finally, we discuss other opportunities for improving the presentation and dissemination of adsorption data, including the introduction of a standard isotherm format, community submissions to the NIST database, and indexing/cataloging of adsorbent materials.