Should We use Argon Isotherms to Characterize the Surface Area of Nanoporous Materials?

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Surface area is one of the most important physical properties of porous material. Generally, surface areas are determined from a nitrogen adsorption isotherm using the Brunauer–Emmett–Teller (BET) method. However, a recent IUPAC report recommends using an argon adsorption isotherm instead of the nitrogen adsorption isotherm to compute the BET surface area due to the purported "orientational" effect [1]. However, the magnitude of such effect has not been fully characterized in the literature, making it difficult for the community to accept the new standard for porous materials characterization. In this study, we carried out large-scale molecular simulations to investigate the orientational effect of nitrogen and its impact on accurately determining the surface area. Molecular simulation results show that the monolayer coverage (obtained directly from the BET analysis) of a material significantly differs between nitrogen and argon adsorption isotherms.