

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

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The Surface area is one of the most important physical properties of porous material. Generally, surface areas are determined from a N₂ adsorption isotherm using the Brunauer–Emmett–Teller (BET) method. However, a recent IUPAC report recommends using an Ar adsorption isotherm instead of the N₂ adsorption isotherm to compute the BET surface area due to the purported “orientational” effect. 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 N₂ and its impact on accurately determining the surface area. The change of the van der Waals interaction between the graphene sheet and gas molecules resulted in a change in the orientation distribution of N₂ on the monolayer. However, when we compared the differences between the true monolayer area and geometric area of N₂ and Ar, There was no significant difference. Finally, we comment on the effect of surface curvature on the orientation of N₂ molecules.