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PoLA (Porosity Local Analysis): An Accurate Descriptor of Microporous Volume to Predict Gas Adsorption in Porous Carbons

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Abstract : A procedure is presented to describe the porosity of microporous solids (e.g., activated carbons): unlike many methods commonly used at present, PoLA (Porosity Local Analysis) is not based on pre-defined pores of regular shape (like spheres or cylinders) but rather on a point-by-point analysis of the inner voids. Then PoLA is particularly suited to describe amorphous porous materials, like carbons, accurately: the procedure can be applied to any atomistic model, and it is much faster than other methods in wide use (for instance, the popular PoreBlazer tool). More importantly, the porous volume distribution provided by PoLA is strongly correlated to gas adsorption isotherms and it can be used to predict the adsorption in new materials effectively. We proved this point by preparing a large dataset of porous carbon models, which were analyzed by PoLA; accurate N2 adsorption isotherms at 77 K were simulated with Grand Canonical Monte Carlo in each model system, and the isotherms were correlated to the porosity distribution by a machine learning (Random Forest) approach. The multiple regression parameters were then used to predict the isotherms in various carbon models, with excellent results. On this basis, PoLA can also be used to deduce the porous volume distribution from experimental nitrogen or argon adsorption isotherms and then predict the performance towards other gases of interest, like hydrogen, methane, or carbon dioxide.

Keywords : gas adsorption isotherms, materials modeling, porous carbons, porous volume distribution
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