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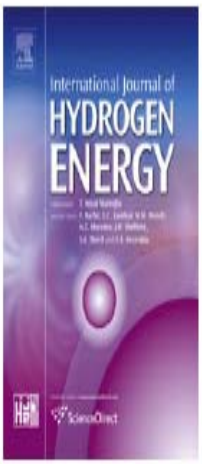

On the application of standard isotherms to hydrogen adsorption in microporous materials

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ABSTRACT

A mathematical framework for simulating equilibrium hydrogen adsorption isotherms in porous materials and estimating the values of key parameters associated with the adsorption process is developed. Explicit expressions for the excess, adsorbed, compressed and absolute masses, for any model isotherm, are derived. The modelling framework is used in combination with five standard equilibrium isotherm models to simulateexperimental data for Prussian blue analogues, nitropussides and metal-organic frameworks *via* nonlinear regression. The surface areas, the affinity and heterogeneity factors, and the pressure-dependent adsorption volumes are calculatedand compared to values available in the literature and the sensitivity of the results to the number of data points is quantified. The consistency of the results using different isotherm models is evaluated.