

Quantum energy levels of hydrogen adsorbed on nanoporous carbons: an intrinsic probe for pore structure, and improving Monte Carlo simulations of adsorption

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Hydrogen is the lightest molecule in nature, making both rotational and translational degrees of freedom eminently quantum mechanical (especially at low temperatures). For isolated molecules the first excited (degenerate) rotational states are at about 175 K above the (non-degenerate) ground state. When the hydrogen molecule is adsorbed, however, interaction with the substrate partially eliminates this degeneracy due to the different adsorption strengths of the different rotational states of the molecule. In this talk, we consider the adsorption of hydrogen in nanometer-size pores in carbon. We show that the rotation-vibration energy levels are strongly dependent on the pore structure (geometry and size). This dependence may be probed by inelastic neutron scattering as a local, non-destructive, probe intrinsic to the system, to characterize nanopores (in fact, using H₂ as the probe makes sure that the pore structure probed is relevant for H₂ adsorption). The rotation-vibration energy levels were also used as input for grand canonical Monte Carlo simulations of H₂ adsorption, improving the accuracy of the simulations.

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