

# Hydrogen Quantum States, Dynamics, and Nanoconfined Melting In Potassium Intercalated Graphite

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Physadsorption of molecular hydrogen followed by a reversible release is a feature of many processes (i.e. gas purification, hydrogen storage, fuel cells, and hydrogenation catalysis). Research on dihydrogen interactions has been further stimulated by the search for materials capable of storing and releasing dihydrogen since these are crucial to a hydrogen economy. An understanding of the interaction of molecular hydrogen with storage materials is needed for the rational design of such materials.

A prototypical material is the family of intercalated graphites where small molecules/atoms intercalate between graphite sheaves and widen the spacing enough for molecular hydrogen to physadsorb. These slit-pore materials allow one to study dihydrogen in confined spaces using volumetric adsorption, molecular dynamics, and neutron scattering. In this study we have made a comprehensive study of hydrogen self- and host-interaction at a range of temperatures (10-120 K). We have identified rotational and translational quantum states and have modeled these using phonon-generated simulated neutron scattering and diffusive scattering from quantum-corrected or delocalized molecular dynamics. We have also modeled hydrogen's hydrodynamics and predict a large elevation of the melting temperature due to nanoconfinement.

At the melting transition we deduce the presence of two types of motions and characteristic lengths/timescales corresponding to short hopping between potassium cages and long-range migration of hydrogen 2D condensed phase clouds. These dynamics have been confirmed with inelastic/quasielastic neutron scattering at a range of temperatures which showed a melting transition, elastic incoherent structure factors, and two disparate length scales in good agreement with molecular simulations.