Surface vibrational states of dispersed platinum catalysts and adsorbed species: computational modelling and inelastic neutron scattering spectra

P.C.H. Mitchell

School of Chemistry, University of Reading, UK

The inelastic neutron scattering (INS) spectra of hydrogen chemisorbed by carbon−supported Pt and Ru catalysts exhibit characteristic riding modes of H on Pt or Ru and H spilled over onto the carbon support. In these riding modes H atoms move in phase with vibrations of the carbon and metal lattices. The lattice modes are amplified by neutron scattering from the H atoms attached to lattice atoms. The carbon vibrational modes observed in the INS spectra were assigned with reference to the INS of a polycyclic aromatic hydrocarbon, coronene, taken as a molecular model of a graphite layer, with the aid of computational modeling. Two forms of spillover hydrogen were identified: H at edge sites of a graphite layer (formed after ambient dissociative chemisorption of H_2), and a weakly bound layer of mobile H atoms (formed by surface diffusion of H atoms after dissociative chemisorption of H_2 at 500 K). The amplification effect of surface vibrational modes via adsorbed hydrogen atoms and hydrogenous species enables the use of inelastic neutron scattering as a technique for studying surface vibrational states of catalyst and other particles.