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**Synergy between Neutron Scattering Experiments and Computational Studies on Sorbates in Porous Materials.** Juergen Eckert, LANSCE-12, Los Alamos National Laboratory, Los Alamos NM 87545, USA, Materials Research Laboratory, Univ. of California, Santa Barbara, CA 93106, USA.

The increasingly close alliance of neutron scattering experiments with computer simulation tools has greatly increased the utility of neutron scattering techniques in many areas of materials chemistry and physics, such as sorbates in porous materials and heterogeneous catalysis. It is the simple nature of the interaction of neutrons with the atomic nuclei that has the consequence that the observations from neutron scattering experiments on condensed phases can readily and accurately be computed. I will describe some examples where elastic and/or inelastic neutron scattering methods have been combined with computational techniques to derive structural details of sorbates in porous materials. These include: simulations of hydrogen in zeolites coupled with a quantum-mechanical analysis of the hindered rotational transitions of the molecule which are accessible by inelastic neutron scattering (INS); detailed comparisons of experimental and simulated INS vibrational spectra of sorbate molecules in zeolites and an organometallic catalyst grafted onto aluminosilicate supports; and the use of differential pair distribution function analysis in neutron diffraction studies of guest-host complexes.

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