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Water diffusion on carbon systems

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The object of this thesis work is the understanding of some properties of water molecules adsorbed on carbon systems, especially graphite. Because of the different polar character, water and carbon do not mix very well, but this system is an excellent model to study spatial confinement of water on hydrophobic substrate in the nanometer scale.
Water and carbon are common and their physics and chemistry has been hugely studied, however the dynamics of water on carbon surfaces is far from being a closed topic.
To explore this system, methods providing both atomic lengthscale and pico- to nanosecond timescale information are crucial for the description of diffusional motion. Those are reachable only with quasi-elastic neutron scattering (QENS) and with quasi-elastic helium atom scattering (QHAS). The application of Neutron Spin Echo spectroscopy on surface diffusion is proved using the spectrometer IN11 in ILL, obtaining directly the real part of the intermediate scattering function. Thermally activated processes are investigated by varying the temperature of the system.
Moreover, simulations are fundamental to analyze experimental results. Force-Field Molecular Dynamics is a tool visualizing directly the motions of the molecules, suggesting then a correct physical interpretation to the neutron scattering results. Coverage- and temperature- dependent intermediate scattering function will be compared with the data-based results in order to establish a diffusion model for water on hydrophobic substrate.

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