Multiscale phenomena in molecular matter



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Neutrons and atomistic simulations to study multiscale phenomena in molecular systems

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Neutron techniques cover many orders of magnitude in time and length scales, which can be extended even further by combining real time and space with reciprocal time and space techniques - neutrons are therefore perfectly suited to studying multiscale phenomena. Since neutrons are scattered primarily by nuclei, the data can be directly compared with atomistic simulations, in particular those based on empirical force fields, which treat electrons implicitly and cover the widest range in time and length scales. A range of examples will be shown on energy and bio-related materials to illustrate how neutrons and atomistic simulations give critical insight into multiscale phenomena in molecular systems.

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