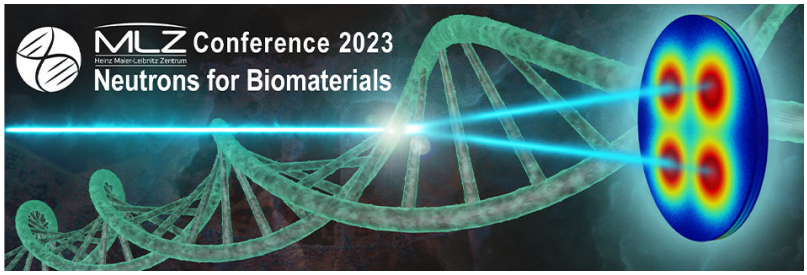

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Challenges in the structure and dynamics of transport in the stratum corneum

Monday 22 May 2023 13:50 (40 minutes)

The outermost layer of mammalian skin, called the stratum corneum (SC), constitutes a self-healing barrier against moisture loss and ingress of foreign substances. The SC comprises flat "bricks" (50-100 micron wide and 1 micron thick corneocytes largely filled with keratins) held together by a 'mortar' of 6-10 layers of lipids (100 nm thick). The corneocytes are hydrophilic, while the lipid matrix is hydrophobic. The ability and way of a chemical to pass the SC is a key point for risk assessment and development of cosmetics.

I will present a realistic multi-scale model with which to study transport through the SC, starting with atomistic simulations on an Angstrom scale and ending with diffusion through the full SC. We explicitly calculate the defected nature of the layered structure between corneocytes and endow it with the local anisotropy such that diffusion across layers differs from diffusion within layers. We study the crossover between transcellular and extracellular transport, as controlled by the relative hydrophobicity (or lipophilicity) of a species, the anisotropic diffusivity within the lipid matrix, the relative mobilities between the lipid matrix and the corneocytes, and the different spatial dimensions of the structure. I will present a number of unanswered questions that could potentially be addressed through neutron scattering, in terms of both structure and dynamics.

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