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Combining the strengths of Neutrons and Molecular dynamics for the study of bio-membranes

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Neutron reflectometry is one of the most powerful methods for investigating the structure of model lipid membranes. These model systems are more easily prepared and experimentally controlled than natural lipid membranes, which are an important integral part of animal and plant cells. In the present work we combine measurements of supported lipid membranes (SLBs) at the MARIA neutron reflectometer and coarse-grained molecular dynamics simulations using the MARTINI force field, for the precise characterization of SLBs at the sub-nanometer scale. The proposed methodology delivers more precise results and should pave the way for studying membranes of a more complex nature, having in mind experiments where membranes interact with bio-molecules, e.g. proteins, small peptides, and nanoparticles that are candidates for drug delivery applications.

Primary author: Dr KOUTSIOUMPAS, Alexandros (JCNS)

Presenter: Dr KOUTSIOUMPAS, Alexandros (JCNS)

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