

# Role of water mediation on biological and non-biological interfaces

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## Abstract

The interactions that water forms with molecules which make up the interfaces of biological and non-biological soft materials play a significant role in the structural and dynamical properties of these interfaces, as well as their interactions with other molecules in their aqueous environment. Recently, my group has combined all-atom molecular dynamics simulations, graph theoretic approaches and machine learning to provide a detailed description of these interactions and how they affect the structure of peptides and various soft interfaces. In this talk, I will discuss how we have used this combination of tools to provide a detailed understanding of how water mediation plays a significant role in the interfacial properties of lipid membranes and polymeric nanoparticles.

## REFERENCES

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