Properties of Confined Water Between two Hydrophilic Surfaces

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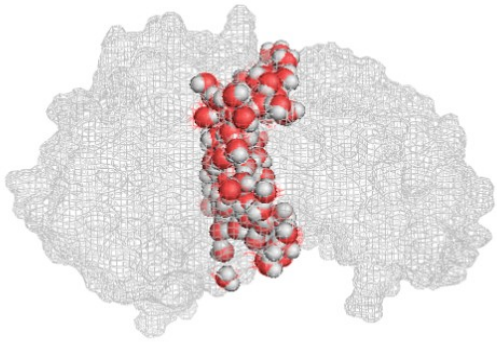

Hydrophilic protein-protein interfaces constitute a major part of protein-protein interfaces and thus are of great importance. However, the qualitative characterization of their association is still an ongoing challenge, and the driving force behind their association remains poorly characterized [1]. Here we present a study of the association of hydrophilic proteins and the role of water through the analysis of extensive molecular-dynamics simulations using three well studied protein complexes: Barnase – Barstar, Cytochrome c – Cytochrome c peroxidase, and the N-terminal domain of enzyme I - Histidine-containing Phosphocarrier protein. We investigated the properties of interfacial water confined between two protein surfaces, which is very important for protein-protein association. The analysis was performed using newly implemented Gromacs plug-ins. Our analysis shows that the confined water between the hydrophilic partners deviates from the bulk values, especially at close separation of the confined proteins.

1. Ulucan Ö, Jaitly T, Helms V. Energetics of hydrophilic protein-protein association and the role of water. *J Chem Theory Comput.,* **2014**, 10, 3512-3524.