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Thermodynamic properties of water solvating biomolecular surfaces[1] MATTHIAS HEYDEN, Ruhr-University Bochum — Changes in the potential energy and entropy of water molecules hydrating biomolecular interfaces play a significant role for biomolecular solubility and association. Free energy perturbation and thermodynamic integration methods allow calculations of free energy differences between two states from simulations. However, these methods are computationally demanding and do not provide insights into individual thermodynamic contributions, i.e. changes in the solvent energy or entropy. Here, we employ methods to spatially resolve distributions of hydration water thermodynamic properties in the vicinity of biomolecular surfaces. This allows direct insights into thermodynamic signatures of the hydration of hydrophobic and hydrophilic solvent accessible sites of proteins and small molecules and comparisons to ideal model surfaces. We correlate dynamic properties of hydration water molecules, i.e. translational and rotational mobility, to their thermodynamics. The latter can be used as a guide to extract thermodynamic information from experimental measurements of site-resolved water dynamics. Further, we study energy-entropy compensations of water at different hydration sites of biomolecular surfaces.

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