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A molecular dynamics study of peptides confined in aqueous nanodroplets and nanofilms

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We carry out molecular dynamics simulations of peptides confined within aqueous nanodroplets and investigate the influence of the temperature-dependent properties of the nanodroplets on peptide folding, localization within the nanodroplet, and secondary structure. Recent computational studies from our group have revealed the emergence of thermodynamic and structural anomalies in liquid water nanodroplets when cooled significantly below the bulk melting temperature. These anomalies impact the distribution of simple ions within the nanodroplets, and here, we extend this exploration to hydrophobic, amphipathic, and hydrophilic peptides.

Our findings reveal an interplay between density and charge structuring in water nanodroplets and the spatial arrangement of charged and polar residues. We examine the dependence of peptide folding propensity on orientation relative to the nanodroplet surface and the disruption of helical secondary structures as subsurface water structure evolves with temperature. To assess the influence of curvature, we conduct comparative studies using confined water nanofilms, and we also simulate peptides in bulk water for comparison.

We quantify the dynamics of water in our systems with a neighbour correlation function, which indicates how long two molecules remain neighbours. Our results reveal slower dynamics within the droplet interior and faster dynamics closer to the surface below a certain temperature. We report on the effect of the different peptides on the dynamics of water.

Keyword-1

Peptide Folding

Keyword-2

Nanodroplets

Keyword-3

Water Dynamics

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