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DNA Hydration: A Perspective from MD Simulations of Solvation Dynamics and Vibrational Spectroscopy

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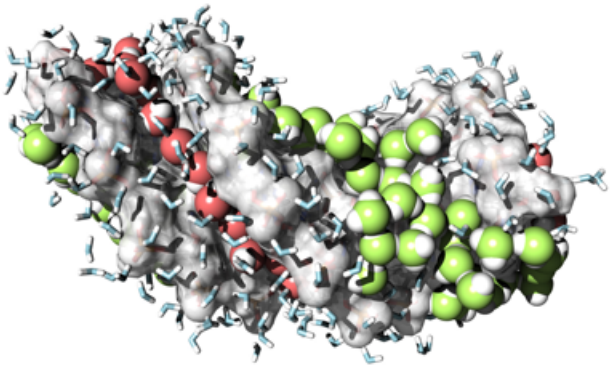
The structure and dynamics of DNA hydration has been elucidated with microsecond-length molecular dynamics (MD) simulations that connect directly with experimental measurements of solvation dynamics in DNA and vibrational spectroscopy of phosphate reporters along the DNA backbone. The experiments provide a superb validation of the simulations, and the simulations provide a molecular-level interpretation of the measurements. Together, the calculations and the experiments reveal a quantitative picture of DNA hydration dynamics in which the orientational dynamics of water is slowed by a factor of 2 – 5 relative to the bulk. This slowing of water dynamics is consistent with other experimental and simulation studies of biomolecular hydration. The simulations also reveal zones of hydration with different structural and dynamical properties. Water in the major and minor grooves of DNA is confined to different degrees, and water in contact with the DNA backbone is perturbed by the negative charge of the sugar-phosphate groups and the positive counterion atmosphere. Each subpopulation has different dynamics that are revealed in the simulations and in the experiments.



Jeudi 28 avril, 14h30
Salle de Séminaire (3ème étage)

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