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VABILO NA PREDAVANJE
V OKVIRU DOKTORSKEGA ŠTUDIJA
KEMIJSKE ZNANOSTI

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z naslovom:

Translational trends in molecular diffusion

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preko spletnega orodja Zoom
https://uni-lj-si.zoom.us/j/92842316999?pwd=WENFOFppUHhJdXVzeVFqNmluRnJUZz09
(Meeting ID: 928 4231 6999, Passcode: 668524)

Vljudno vabljeni!

Abstract:

Abstract: Common kinetic models for molecular diffusion involve variations of the Stokes-Einstein relation. In applying such models, the diffusion of differing molecules in similar environments is primarily distinguished by the unique molecular weights, which can be used to approximate the hydrodynamic radii of the microscopic particles. While general in form, such mass-based predictions are of limited accuracy without extensive statistical fitting and/or corrections for shape and bound solvent. In this presentation, I will introduce the history of predicting translational diffusion of microscopic systems and how we can make accurate estimations with computational molecular simulations. This leads to an alternate look at the fundamental physical interactions that govern dynamics in biomolecular systems, and it provides a foundation for a method of assembling the hydrodynamic radii of protein systems using the component diffusive behavior of individual amino acids. We use this approach to accurately predict diffusion coefficients of small peptides as well as individual proteins and protein assemblies of various size. This work also shows how and why some molecules exhibit distinctly different translational diffusion behavior despite having nearly identical masses.