Curriculum Vitae

Name
Jochen S Hub

Current Position
Professor for Theoretical Biophysics, Saarland University, Germany

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Education & Professional Experiences (Times New Roman, 11 point)
2018–: Full Professor (W3), Saarland University, Germany
2017–2018: Junior group leader (Emmy Noether and Heisenberg programmes by the DFG), University of Göttingen, Germany
2009–2011: Marie-Curie fellow, Uppsala University, Sweden
2008–2009: Postdoc, Max-Planck-Institute for Biophysical Chemistry, Göttingen, Germany
2008: PhD, Max-Planck-Institute for Biophysical Chemistry, Göttingen, Germany
1998–2004: Physics studies at Universities of Stuttgart (Germany) and University of Oregon

Research Interests (Times New Roman, 11 point)
Interpretation of small-angle scattering data using molecular dynamics simulations
Membrane biophysics, topological transitions of membranes
Computational drug discovery

Selected Publications (※3-5 major papers)
Depletion of the protein hydration shell with increasing temperature observed by small-angle X-ray scattering and molecular simulations. Linse, Cho, Scotte, Anfinrud, Hub, *J Am Chem Soc* 147, 47117-47125 (2025)
How pore formation in complex biological membranes is governed by lipid composition, mechanics, and lateral sorting. Starke, Allolio, Hub, *PNAS Nexus*, 4, pgaf033 (2025)
Structural insights into tecovirimat antiviral activity and poxvirus resistance. Vernuccio, Martínez León, …, Hub, Guardado-Calvo, *Nat Microbiol* **10**, 734–748 (2025)
BindFlow: A Free, User-Friendly Pipeline for Absolute Binding Free Energy Calculations Using Free Energy Perturbation or MM(PB/GB)SA. Martínez León, Andersen, Hub *J Chem Theory Comput* 22, 1198-1213 (2026)

Lecture Title
From nuisance to knowledge: learning hydration shell structure from SAXS and SANS using explicit-solvent MD simulations

Abstract (500 words maximum)

The hydration shell is an integral part of proteins since it plays key roles in folding, conformational transitions, and molecular recognition. These effects are particularly important for intrinsically disordered proteins and misfolded states, where extended and heterogeneous conformations expose large surface areas to solvent and couple conformational

equilibria to hydration. While the dynamics of the hydration shell have been described in detail by spectroscopic techniques, its structure remains less understood due to the lack of hydration shell-sensitive structural probes with high spatial resolution. Whether MD simulations correctly reproduce hydration shell structure is not well established. Small-angle scattering (SAS) with X-rays or neutrons (SAXS/SANS) is sensitive to the hydration shell; however, hydration effects have traditionally been treated as nuisance parameters rather than as structural observables. Here, we combine SAS data with MD simulations and explicit-solvent SAS predictions to reveal how surface properties, temperature, and force fields influence protein hydration. We find that (i) MD simulations with certain force fields yield excellent agreement with SAS data, while others do not; (ii) chemical characteristics of exposed surface regions strongly modulate hydration shell structure; and (iii) temperature-dependent SAXS and MD consistently show that the hydration shell is remarkably temperature-sensitive. Our results establish the combination of SAS and explicit-solvent MD simulations as a quantitative structural probe of protein hydration.