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Solvation Shells and Simulation Cells: Advances in modeling X-ray Solution Scattering for Time-Resolved Studies

Thursday, June 26, 2025 5:20 PM (20 minutes)

The role of the solvent in ultrafast processes has become a focus of interest for many researchers within femtochemistry and beyond. To interpret emerging time-resolved x-ray scattering experiments, we therefore need forward models that accurately predict scattering across the full range of momentum transfer, q. This talk will present new methods to correct finite simulation cell errors in scattering signals calculated from molecular dynamics simulations[1], particularly at low values of q, improving the accuracy of forward models for the solvation structure of solvated systems. Our renormalization scheme, based on excluded volume corrections to radial distribution functions, recovers the correct q = 0 limit. The work also provides practical guidance for integrating MD simulations into experimental structural studies.
To accurately predict the coupling between solute and solvent, we present an analysis of the nature of the interactions governing solvent structure, to guide future strategies for accurate simulations[2]. Lastly, for molecules with significant conformational flexibility, we show how to employ robust conformational sampling techniques to assist the structural modeling of picosecond-timescale excited-state conformational dynamics of an all-organic covalent dimer, which was very recently recorded at the European XFEL.

[1]:Dohn, A. O.; Markmann, V.; Nimmrich, A.; Haldrup, K.; Møller, K. B.; Nielsen, M. M. Eliminating Finite-Size Effects on the Calculation of x-Ray Scattering from Molecular Dynamics Simulations. The Journal of Chemical Physics, 2023, 159. https://doi.org/10.1063/5.0164365.

[2] Zulfikri, H.; Pápai, M.; Dohn, A. O.; Simulating the solvation structure of low- and high-spin [Fe(bpy)3]2+: long-range dispersion and many-body effects. Physical Chemistry, Chemical Physics, 2022, 14. https://doi.org/10.1039/d2cp00892k

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