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Proteins meet colloid physics: The importance of hydrodynamics, polydispersity and patchiness - new possibilities with neutron spectroscopy

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Diffusion of proteins is essential for transport and regulation in biology. Changes in the short time diffusion - where hydrodynamic and electrostatic interactions dominate whilst protein-protein collisions can be neglected - influence the long time diffusion. For monodisperse protein solutions, systematic studies in the short-time regime confirm a comprehensive picture in good agreement with colloid theory, describing the dependence on temperature, size, and volume fraction [1-3]. In contrast, biological systems contain differently sized particles in the solution. This polydisperse crowded environment influences the diffusion of individual tracers, depending on their size. Recently, the short-time diffusion of tracer proteins has been investigated in the presence of a naturally crowded environment both with quasielastic neutron backscattering and simulations, confirming a good agreement between experiment and model [4]. The simulations as well as further studies [5] showed that the short time diffusion of the tracers changes if the environment changes from a purely monodisperse to a polydisperse environment. Moreover, neutron backscattering spectroscopy on solutions containing proteins with two distinct hydrodynamic radii, namely bovine serum albumin (BSA) and immunoglobulin (IgG), provides additional access to the situation of differently sized tracers [6]. By changing both the total volume fraction as well as the fraction of BSA and by applying fits along energy and momentum transfer simultaneously, the global diffusion of both proteins can be separated from the internal diffusion and from the solvent contribution. The resulting diffusion coefficients for both proteins are in quantitative agreement with the predicted deviation from the monodisperse case of pure BSA and pure IgG, respectively. The methods developed also benefit systematic studies of protein cluster formation, including crowding- and salt-induced clusters [7-11], where the latter can be modeled as patchy colloids, as well as clusters of monoclonal antibodies [12]. References: [1] M.Grimaldo et al., Quart.Rev.Biophys. 52, e7 (2019), https://doi.org/10.1017/S0033583519000027 [2] M.Grimaldo et al., J.Phys.Chem.B 118, 7203 (2014), https://doi.org/10.1021/jp504135z [3] F.Roosen-Runge et al., PNAS 108, 11815 (2011), https://doi.org/10.1073/pnas.1107287108 [4] M.Grimaldo et al., J.Phys.Chem.Lett. 10, 1709 (2019), https://doi.org/10.1021/acs.jpclett.9b00345 [5] M.Wang et al., J.Chem.Phys. 142, 094901 (2015), https://doi.org/10.1063/1.4913518 [6] C.Beck et al., J.Phys.Chem.B 126, 7400 (2022), https://doi.org/10.1021/acs.jpcb.2c02380 [7] M.Braun et al., J.Phys.Chem.Lett. 8, 2590 (2017), https://doi.org/10.1021/acs.jpclett.7b00658 [8] C.Beck et al., J.Phys.Chem.B 122, 8343 (2018), https://doi.org/10.1021/acs.jpcb.8b04349 [9] F.Roosen-Runge et al., Sci.Rep.4, 7016 (2014), https://doi.org/10.1038/srep07016 [10] M.Grimaldo et al., J.Phys.Chem.Lett. 6, 2577 (2015), https://doi.org/10.1021/acs.jpclett.5b [11] C.Beck et al., Soft Matter 17, 8506 (2021), https://doi.org/10.1039/D1SM00418B [12] I.Mosca et al., Mol.Pharm. 20, 4698 (2023), https://doi.org/10.1021/acs.molpharmaceut.3c00440

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