frontiers | Frontiers in Soft Matter

TYPE Editorial
PUBLISHED 09 January 2025
DOI 10.3389/frsfm.2024.1548411

OPEN ACCESS

EDITED AND REVIEWED BY
Raffaele Mezzenga,
ETH Zürich, Switzerland

*CORRESPONDENCE
Tommy Nylander,
tommy.nylander@fkem1.lu.se

RECEIVED 19 December 2024
ACCEPTED 30 December 2024
PUBLISHED 09 January 2025

CITATION
Nylander T (2025) Editorial: Editors' showcase 2023: self-assembly and self-organisation.
Front. Soft Matter 4:1548411.
doi: 10.3389/frsfm.2024.1548411

Editorial: Editors' showcase 2023: self-assembly and self-organisation

Tommy Nylander*

Physical Chemistry, Department of Chemistry, Lund University, Lund, Sweden

KEYWORDS

lipids, self-assembly, drug delivery, cellulose, coarse graining, fuid dynamics

Editorial on the Research Topic
Editorial: Editors' showcase 2023: self-assembly and self-organisation

This Research Topic deals with key aspects of Self-Assembly and Self-Organisation in biomimetic and soft matter structures of relevance for application in and function of biological systems. This involves modelling of the systems by coarse graining (Banerjee et al.), the preparation of porous biopolymeric scaffold for potential use in tissue repair (Chen and Andrews), self-assembled systems for delivery of probiotics and enzymes (Risbo et al.) as well as the flow of complex biological fluids and how that is affected by the composition (Herrera-Valencia et al.). The common denominators of these studies are the influence of the self-assembly structure and how this can be manipulated by the composition and different fundamental forces. In case of amphiphilic molecules the formed structures that control the cavities can be understood in terms the balance of the length (L) and volume of the hydrocarbon chain (v) and size polar head group expressed as the head group area (a) formulated as the packing parameter (v/aL) in the 1970s (Israelachvili et al., 1976; Mitchell and Ninham, 1981). The same principles can be applied to more complex and macromolecular systems. Regarding the forces involved, the classical DLVO theory that involves the attractive van der Waals forces and repulsive electrostatic interactions have its shortcomings in describing colloidal systems and proteins as it does not consider, e.g., the hydrophobic effect and specific ion effects (Salis and Ninham, 2014). Direct measurements of the force between hydrophobic surfaces in aqueous solutions has helped us to understand the nature and range of the interaction, but modelling is still challenging (Meyer et al., 2006).

Different coarse-graining approaches are available and provides the means to model the process of self-assembly of biomolecules and can cover different spatiotemporal scales (Banerjee et al.). This involves both top-down and bottom-up approaches, where covering large length scales means compromising on resolution. As with all modelling accurate experimental data to verify the model and the force field is needed.

Scaffolds for tissue repair can be built using self-assembly, where the use of cellulose nanocrystals (CNC) enable a way to tune the porosity of the material (Chen and Andrews). An interesting approach to control crystallinity of the system is to use freeze-casting of carboxylated cellulose nanocrystals and together with CNC with attached magnetite nanoparticles, macropore morphology can be controlled by temperature and magnetic field.

Food is a complex soft matter that is self-assembled from a range compounds like proteins, lipids, and carbohydrates into hierarchical structures at multiple length scales that

controls the impact on human health and wellbeing (Risbo et al.). The uptake of nutrients relies on a healthy gastrointestinal tract and its microbiome. For this purpose, probiotic bacteria and enzymes can be delivered to the intestinal system by formulated with lipids, carbohydrate and proteins using self-assembly principles.

Another import physiological aspect is the flow of biological fluids in, e.g., the blood vessels that can be described and modelled as an electro-osmotic phenomenon (Herrera-Valencia et al.). Such modelling, emulating, e.g., blood with varying cholesterol levels, must account for (colloidal) interactions within the fluid in addition rheology and fluid dynamics. The knowledge gain will be important for the diagnosis of certain pathology conditions that depends on the cholesterol level.

For many years the effect of added salt and/or buffers was not fully taken into account or even ignored. The influence of specific ions on self-assembly structures and interaction forces as qualitatively predicted the Hofmeister Series, is important for phenomena in the medicine, biology, food, soft matter as well as for a range of industrial applications. As pointed out by Gregory et al. (2022) there is still a lack of a general predictive theory that can be applied across different systems. This is partly due to the complexity of real systems that involves a multitude of components including both the ions and the specific counterions as well as the solvent and possibly also co-solutes. Here more experimental studies as well as more detailed and predictive theoretical modelling is needed.

Author contributions

TN: Writing–original draft, Writing–review and editing.

Funding

The author(s) declare that financial support was received for the research, authorship, and/or publication of this article. Funding from the Swedish Research Council (Vetenskapsrådet) (grant number 2020-05421).

Conflict of interest

The author declares that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

The author(s) declared that they were an editorial board member of Frontiers, at the time of submission. This had no impact on the peer review process and the final decision.

Generative AI statement

The author(s) declare that no Generative AI was used in the creation of this manuscript.

Publisher's note

References

Gregory, K. P., Elliott, G. R., Robertson, H., Kumar, A., Wanless, E. J., Webber, G. B., et al. (2022). Understanding specific ion effects and the Hofmeister series Hofmeister series. *Phys. Chem. Chem. Phys.* 24, 12682–12718. doi:10.1039/d2cp00847e

Israelachvili, J. N., Mitchell, D. J., and Ninham, B. W. (1976). Theory of self-assembly of hydrocarbon amphiphiles into micelles and bilayers. *J. Chem. Soc. Faraday Trans. 2 Mol. Chem. Phys.* 72, 1525–1568. doi:10.1039/f29767201525

Meyer, E. E., Rosenberg, K. J., and Jacob Israelachvili, J. (2006). Recent progress in understanding hydrophobic interactions. *PNAS* 103, 15739–15746. doi:10.1073/pnas.0606422103

Mitchell, D. J., and Ninham, B. W. (1981). Micelles, vesicles and microemulsions. *J. Chem. Soc. Faraday Trans. 2 Mol. Chem. Phys.* 77, 601–629. doi:10.1039/f29817700601

Salis, A., and Ninham, B. W. (2014). Models and mechanisms of Hofmeister effects in electrolyte solutions, and colloid and protein systems revisited. *Chem. Soc. Rev.* 43, 7358–7377. doi:10.1039/c4cs00144c