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Behavior of Charged Polymer Chains in Solution and Adsorption Processes

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Abstract: This research article investigates the influence of electrostatic interactions on the processes of self-organisation, adsorption, and complex formation within polyelectrolyte and polyampholyte systems. The study was conducted employing molecular dynamics simulation methods to rigorously analyse the conformational states of charged macromolecules in solution, their specific aggregation patterns, and their interaction mechanisms with oppositely charged surfaces. The findings demonstrate that the intricate equilibrium between long-range electrostatic forces and short-range molecular attraction fundamentally determines the structural configuration and functional attributes of polymer systems. Furthermore, the scientific insights obtained in this study carry significant importance for the design of advanced drug delivery systems and the engineering of novel functional materials.

Keywords: Polyelectrolytes, polyampholytes, microgels, adsorption, electrostatic interaction, molecular dynamics.

INTRODUCTION:

Polyelectrolytes represent a fundamental class of macromolecules that occupy a central role in contemporary chemistry and materials science, primarily due to their unique capacity to undergo dissociation in polar solvents and subsequently generate charged groups along the polymer backbone [1]. Within such complex systems, the dynamic competition and intricate interplay between long-range electrostatic repulsion forces and short-range molecular attraction forces lead to sophisticated structural transitions and phase behaviours [2]. As a direct consequence of these internal interactions, polyelectrolyte chains adopt a variety of distinct conformational states, ranging from highly extended configurations to compact globular and clustered architectures [3].

A significant number of essential biological macromolecules, most notably proteins and various nucleic acids, inherently exhibit polyelectrolyte characteristics, which substantially broadens their scope of application in the field of biomedicine [4]. In particular, these properties are increasingly being exploited to develop advanced drug delivery vehicles and targeted carrier systems [5]. Furthermore, polyampholytes are distinguished by the simultaneous presence of both positively and negatively charged functional groups within their molecular structure; their specific conformational behaviour is profoundly influenced by the pH value of the surrounding aqueous environment [6]. This stimuli-responsive characteristic provides a robust mechanism for employing polyampholyte systems as highly controlled and programmable drug release platforms [7]. Consequently, a detailed investigation into the fundamental physical nature of electrostatic interactions and their overarching role in governing the behaviour of polymer systems remains a critical and highly relevant scientific endeavour.

METHODOLOGY

This research is specifically focused on the investigation of physical and chemical processes at the molecular level, with all primary computations performed using the molecular dynamics (MD) simulation method. The modelling procedures were executed utilizing the high-performance, open-source software package LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). Within the scope of this study, linear polyelectrolyte chains, corresponding counterions, polyampholyte microgels, and various charged particles were employed as representative model systems.

The interactions between the constituent particles were rigorously characterised through the following mathematical models:

– Short-range van der Waals forces were defined using the Lennard-Jones potential, which effectively describes the repulsion and attraction between non-bonded atoms.

– Covalent bonds within the polymer backbones were modelled using the FENE (Finite Extensible Nonlinear Elastic) potential, ensuring realistic chain flexibility and stretch limits.

– Long-range electrostatic interactions were computed via the PPPM (particle–particle/particle–mesh) solver, which provides high-precision accounting of Coulombic forces in periodic systems.

The critical system parameters selected for analysis included the degree of macromolecular charge, particle dimensions, and varying solvent conditions. The processing of raw computational data and subsequent statistical analysis were carried out using bespoke algorithms developed in Java, Python, and C++ programming languages. Due to the significant computational intensity of these simulations, large-scale tasks were performed on the high-performance computing clusters — the "Lomonosov" and "Lomonosov-2" supercomputers at the M.V. Lomonosov Moscow State University.

The application of this robust methodology allows for the high-resolution examination of both the structural configurations and dynamic properties of complex charged polymer systems.

MAIN PART

In polyelectrolyte systems, electrostatic interactions play a fundamental role in the spatial organisation and structural evolution of polymer chains. The delicate equilibrium between the electrostatic repulsion of similarly charged groups and short-range attractive forces results in the formation of diverse structural states. Research indicates that:

– At low charge densities, polymer chains predominantly aggregate to form spherical clusters.

– As the degree of charge increases, the repulsive forces between the chains intensify, leading to a significant reduction in the degree of aggregation.

– Under specific physico-chemical conditions, the formation of more complex, cylindrical clusters has been observed.

The quality of the solvent also acts as a critical determining factor; a deterioration in solvent quality enhances intermolecular attractive forces, thereby accelerating the aggregation process. Simultaneously, the interaction of polyelectrolyte chains with oppositely charged surfaces facilitates the process of adsorption. While adsorption is primarily driven by electrostatic attraction, the introduction of salt into the solution causes the screening of these electrostatic forces. This screening effect leads to the detachment of the chains from the surface, a phenomenon known as the desorption process.

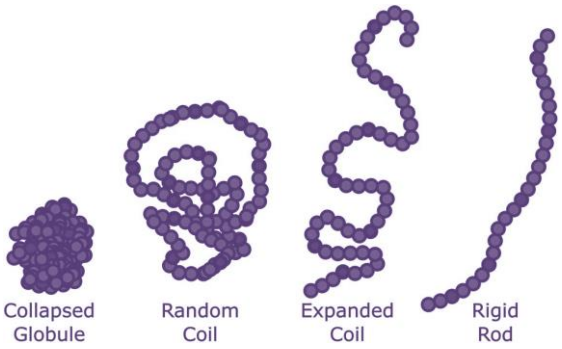

Figure 1. Conformational states of polyelectrolyte chains as a function of solvent quality and electrostatic interactions.

Polyampholyte Microgels and the "Trap" Effect

Polyampholyte microgels represent even more intricate systems, where their dynamic behaviour is intricately linked to the precise distribution of charges and the pH of the medium. In microgel systems characterised by a random charge distribution, molecules are typically released into the surrounding medium at a rapid rate. Conversely, in microgels possessing a distinct core-shell architecture, molecules can become entrapped within the internal cavity. This phenomenon is scientifically attributed to the electrostatic “trap” effect, which is essential for developing controlled-release technologies.

RESULTS

The results of the investigations conducted demonstrate that electrostatic interactions play a decisive role in the structural and dynamic evolution of both polyelectrolyte and polyampholyte systems. It was established that the behaviour of polyelectrolyte chains in solution is directly contingent upon their specific charge density and the thermodynamic quality of the solvent. The following key observations were made:

− At low charge densities, the polymer chains tend to self-assemble into spherical aggregates due to dominant attractive forces.

− As the degree of charge increases, electrostatic repulsion forces begin to prevail, leading to a marked reduction in the degree of aggregation.

− Under specific environmental conditions, the formation of elongated, cylindrical clusters was explicitly observed.

− A deterioration in solvent quality was found to significantly enhance the aggregation process, resulting in the emergence of complex spatial architectures within the system.

Furthermore, the interaction of polyelectrolyte chains with oppositely charged surfaces confirmed that the adsorption process is primarily driven by electrostatic attraction. The study also revealed that:

− The introduction of salt into the solution environment screens the electrostatic interactions, effectively triggering the detachment of chains from the surface, a process known as desorption.

− The findings indicated that the salt concentration required to induce surface desorption is substantially higher than the concentration necessary for the dissociation of interchain complexes.

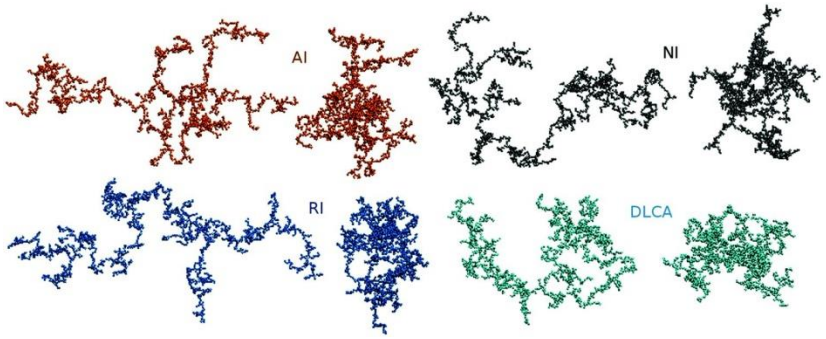

Figure 2. Structural configurations of polyelectrolyte aggregates formed under various physical parameters.

In the case of polyampholyte microgels, the system behaviour was found to vary significantly in response to the pH value of the medium. At high or low pH levels, the microgels remain in a highly charged state, resulting in an expanded conformation due to internal repulsion. Conversely, at intermediate pH values (near the isoelectric point), the microgels transition into a collapsed or compacted state. Additionally, the capacity of these microgels to capture and subsequently release charged protein molecules was quantified, demonstrating that such processes can be precisely regulated via pH adjustment. Observations showed that while molecules are released rapidly in microgels with a random charge distribution, they tend to be sequestered within the interior of core-shell structures due to the electrostatic “trap” effect.

Overall, the obtained results highlight that electrostatic interactions are the primary factor defining the structural and functional attributes of polymer systems, confirming the feasibility of controlling these systems by modulating external environmental conditions.

CONCLUSION

The findings of this comprehensive study demonstrate that electrostatic interactions constitute one of the primary factors determining the structural organisation and functional characteristics of polyelectrolyte and polyampholyte systems. It was observed that the aggregation of polyelectrolyte chains in solution is directly contingent upon both their degree of charge and the thermodynamic quality of the solvent. As these parameters fluctuate, the macromolecules transition between the formation of spherical or cylindrical structures and existing in a free, non-aggregated state.

Furthermore, the investigation established that the interaction of polyelectrolyte chains with oppositely charged surfaces leads to the initiation of the adsorption process, which is fundamentally governed by electrostatic attractive forces. The study revealed that:

− The addition of salt to the solution leads to the screening of electrostatic interactions, thereby triggering desorption.

− The salt concentration required for successful desorption from a surface is notably higher than the concentration necessary for the dissociation of interchain complexes.

In the context of polyampholyte microgel systems, the pH value of the environment emerges as the primary regulatory factor. The resulting redistribution of charges significantly alters the volume and structural conformation of the microgels. This mechanism provides a precise means of controlling their capacity to capture and release charged molecules. Notably, the specific character of charge distribution was found to have a substantial impact on the rate of molecular release, with the electrostatic “trap” effect being particularly prominent within core-shell architectures.

In summary, the results obtained confirm the potential to manipulate the behaviour of polymer systems through the strategic modulation of electrostatic interactions. These scientific conclusions serve as a critical theoretical and practical foundation

for the synthesis of novel functional materials, as well as the development of advanced systems for targeted drug delivery and controlled pharmaceutical release.

REFERENCES

1. Dobrynin, A. V. (2020). Polyelectrolytes: On the doorsteps of the second century. Polymer (Guildf), 202, 122714.
2. Thünemann, A. F., Müller, M., Dautzenberg, H., Joanny, J. F., & Löwen, H. (2004). Polyelectrolyte Complexes. Advances in Polymer Science, 166, 113–171.
3. Yaroslavov, A. A., Sybachin, A. V., & Efimova, A. A. (2018). Stabilization of electrostatic polymer-colloid complexes. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 558, 1–7.
4. Müller, M. (Ed.). (2014). Polyelectrolyte Complexes in the Dispersed and Solid State I (Vol. 255). Springer Berlin Heidelberg.
5. Morin-Crini, N., Lichtfouse, E., Torri, G., & Crini, G. (2019). Applications of chitosan in food, pharmaceuticals, medicine, cosmetics, agriculture, textiles, pulp and paper, biotechnology, and environmental chemistry. Environmental Chemistry Letters, 17(4), 1667–1692.
6. Jeon, J., & Dobrynin, A. V. (2006). Molecular Dynamics Simulations of Polyelectrolyte−Polyampholyte Complexes. Effect of Solvent Quality and Salt Concentration. The Journal of Physical Chemistry B, 110(48), 24652–24665.
7. Ogawa, K., Nakayama, A., & Kokufuta, E. (2003). Preparation and Characterization of Thermosensitive Polyampholyte Nanogels. Langmuir, 19(8), 3178–3184.