Universal shape properties of mesoscopic polymer chains, polymer stars and their aggregates

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We analyse macromolecular shape by the dissipative particle dynamics simulations. In the **case study A** we discuss a single linear chain in a good solvent and examine its asphericity, prolateness, size ratio and their probability distributions. Good agreement is achieved with available theoretical and simulation results. In the **case study B** we extend our analysis to the single homo- and hetero-stars immersed in a solvent of variable quality [2]. Asphericity and related properties are examined at various arms compositions as the functions of solvent quality. For the homo-star, the asphericity maximum is found close to the θ-point condition explained by the interplay between the enthalpic and entropic contributions to the free energy. In the **case study C** we consider the changes in shape-related universal ratios for a homo-star and for its individual arms with the increase of the number of arms f. The results for the universal ratios show very good agreement with the available data from the Monte Carlo and molecular dynamics simulations [3], whereas some of the ratios are calculated for the first time. In the **case study D** we looked at the aggregation of the amphiphilic stars in a solvent [4]. Four architectures are examined: the miktoarm star, two different diblock stars and a set of four disjoint linear diblock copolymers. We observed four different shapes of aggregats: spherical, rod-like and disc-like micelles and a spherical vesicle. The change from a spherical to aspherical micelle shape is monotonous, whereas that from an aspherical micelle into a spherical vesicle is found to be discontinuous.

[1]. O. Kalyuzhnyi, Ja. Ilnytskyi, Yu. Holovatch, C. von Ferber, *J. Phys.: Cond. Matt.* **28** (2016) 505101.

[2] O. Kalyuzhnyi, Ja. Ilnytskyi, Yu. Holovatch, C. von Ferber, *J. Phys.: Cond. Matt.* **30** (2018) 215101.

[3] O. Kalyuzhnyi, K. Haidukivska, V. Blavatska, Ja. Ilnytskyi, *Macromolecular Theory and Simulations*, accepted on 9-th of April 2019.

[4]. O. Kalyuzhnyi, Ja. Ilnytskyi, C. von Ferber, *Condens. Matter Phys.* **20** (2017) 13802.