"Atomistic Simulations of Poly(Dimethylsiloxane) and Poly(Lactic Acid) Polymer Systems for Directed Self-Assembly Applications"

Lithography has been the most important technology that has revolutionized the semiconductor and data storage industry and it is used in the fabrication of integrated circuits and microchips. However, conventional semiconductor lithography techniques become very expensive and inefficient when the feature size that has to be patterned is less than 30nm. In order to cross the Rubicon of the scale miniaturization, alternative methods should be studied and considered. One of the most promising and potential candidates is the Directed Self Assembly of Block Copolymers. In order to guide the selection of the most suitable Block Copolymers for Directed Self Assembly applications, apart from experimental work there is also an urgent need of computational as well.

The Poly(Dimethylsiloxane)-b-Poly(Lactic acid) (PDMS-b-PLA) block copolymer is considered to be very suitable for directed self-assembly applications due to its ability to self-organize easily into tiny domains. A thermodynamic factor that describes the appearance of order from disorder is the Flory-Huggins interaction parameter χ. The PDMS-b-PLA appears to have a value of χ significantly higher than other block copolymers, and thus, it will possibly enhance the Directed Self Assembly of Block Copolymers for Lithography purposes. At this work, a lot of attention is paid to estimate the χ parameter of the PDMS-b-PLA. Apart from that, other volumetric, dynamical, solubility and conformational properties of PDMS and PLA have been computationally studied by different simulation methods and will be presented as well.