הטכניון - מכון טכנולוגי לישראל

TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY

הפקולטה להנדסה כימית
ע"ש וולפסון
The Wolfson Department of Chemical Engineering

Wolfson Department of Chemical Engineering Seminar

Lecture Hall 6, Wolfson Department of Chemical Engineering,

October 21, 2015, Wednesday, 13:30

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Structural investigation of Ca-Alginate physical gelation using molecular dynamics simulation

Calcium alginate is a natural occurring gel composed of two basic monomer units (guluronic (G) and mannuronic (M)). Calcium alginate gel is a useful and very popular material for novel medical applications such as immobilization matrix device for drug delivery systems. G monomers forms specific strong physical cross-links with the calcium ions to form a gel, but M monomers plays an important role in gel formation as well. The lack of definitive models for alginate structure-behavior relations drives the use of Molecular Dynamics simulation to provide theoretical prediction and better understanding of the alginate gelation mechanisms, gel nanostructure and physical properties relationships in alginate gels. We model the Ca-alginate physical gelation process by addition of Ca ions in different concentrations to a known G/M monomer sequence Na-alginate solution and investigate the chain association mechanisms, addressing the different models that describe alginate gel microstructure such as the "egg-box" model, dimerization, lateral association, multiple junction zones, stiff vs. flexible zones and "broken rod". We investigated structural characteristics of Ca-alginate polymer chains such as gyration radii, persistence length and end-to-end distance in dependence of the G/M composition and in comparison to known theoretical polymer chains models. We find that association between chains is more favorable in the following alginate composition order GMM>GMGM>MMM>GGG>GGM, which is also related to the gradual chains stiffness that was found to be as follows GGG>MMM>GGM>GMGM>GMM and the role of M monomers as elasticity moderators.

Refreshments served at 13:15