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In silico study of the self-assembly and gelation of sugar derivatives

Dafna Knani
ORT Braude College, Israel

Low molecular weight gelators are molecules capable of forming gels in which they are self-assembled into a physical 3D network of fibers, held together by non-covalent interactions like hydrogen bonds, Van der Waals forces and π–π-interactions. The organic gelator 1,3 (R):2,4(S)-dibenzylidene-D-sorbitol (DBS) self-organizes to form a 3-D network at relatively low concentrations in a variety of nonpolar organic solvents and polymer melt. DBS could be transformed into a hydrogelator by introduction of hydrophilic groups, which facilitate its self-assembly in aqueous medium. In this work, the self-assembly of DBS and its derivatives was investigated by molecular modeling. A dynamic molecular simulation was carried out using atomistic and quantum tools included in the Material Studio 8.0 (by Biovia) software. Various properties (cohesive energy density, mixing energy, radial distribution function) were calculated to illustrate the interactions that govern the self-assembly of the examined compounds. The results of the simulation indicate that the interaction between DBS-COOH molecules is stronger than DBS-$CONHNH_2$ and DBS and its water compatibility is highest. Therefore, DBS-COOH seems to be a better hydrogelator than DBS-$CONHNH_2$ and DBS. Intermolecular H-bonding interactions are formed between the three molecules as pure substances and they dramatically decrease in the presence of water. In contrast, the intra-molecular interactions increase in water. This result indicates that in aqueous environment the molecular structure tends to be more rigid and fixed in the preferred conformation. Due to H-bonds, DBS and its derivatives form a rigid structure which might explain their tendency to create nanofibrils. In order to obtain effective hydrogelators, fine-tuning of the balance between the hydrophilic (soluble) and hydrophobic (insoluble) parts is essential.

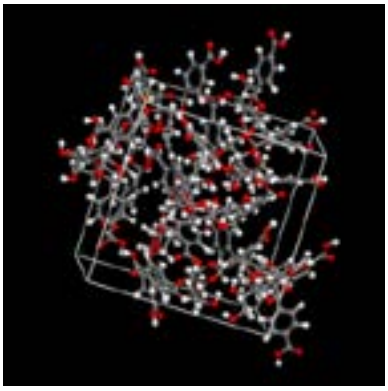

Figure: Periodic cubic cell of DBSCOOH, after 500ps dynamic simulation

Recent Publications

1. D Alperstein, D Knani, N Borchmann, M Spekowius and C Hopmann (2014) Prediction of environmental stress cracking in polycarbonate by molecular modeling, Polymers for Advanced Technologies 25:1433-1438
2. D Knani, D Alperstein, Th Kauth, D Kaltbeitzel and Ch Hopmann (2015) Molecular modeling study of CO_2 plasticization and sorption onto absorbable polyesters, Polymer Bulletin 72(6):1467-1486
3. D Alperstein and D Knani (2017) Design of novel plasticizers for nylon: from molecular modeling to experimental verification, Polymers for Advanced Technologies 28(1):53-58
4. D Knani, Hilla Barkay-Olami, David Alperstein and Meital Zilberman (2017) Simulation of novel soy protein-based systems for tissue regeneration applications, Polymers for Advanced Technologies, 28(4), 496–505
5. D Knani and D Alperstein (2017) Simulation of DBS, DBS-COOH and DBS-$CONHNH_2$ as hydrogelators. The Journal of Physical Chemistry Part A 121(5):1113-1120.

Biography

Dafna Knani is a Senior Lecturer in the Department of Biotechnology Engineering at ORT Braude College. Currently, she is the Head of MSc program in Biotechnology. She is an Organic Polymer Chemist. She has completed her Graduation in the Faculty of Chemistry at Technion-Israel Institute of Technology. In the past, she worked for surgical bio-polymeric materials start-up company (developing adhesives for hard tissues) and as a Research Chemist and Project Leader at Israel Chemicals Ltd. Her current research focuses on "Molecular modeling of materials and biomaterials, especially simulation of systems used for controlled drug release and tissue engineering".

dknani@braude.ac.il

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