Computational Design of Water-Mediated Interactions

M. Scott Shell
Myers Founders Chair Professor
Vice Chair of Chemical Engineering
University of California, Santa Barbara

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Abstract:

Hydrophobic interactions are a fundamental driving force for self-organization and self-assembly in biology, and key players in the production and performance of many synthetic materials. From a theoretical point of view, both hydrophobic solvation and interactions have been studied extensively for model solutes and interfaces. However, many molecules of interest are highly heterogeneous in both chemistry (e.g., with both hydrophobic and hydrophilic groups) and conformations (e.g., through configurational fluctuations). Such heterogeneities produce a rich potential design space that can be leveraged to create surfaces and solutes with optimized thermophysical behaviors. In this talk, I discuss our recent work to understand and to design heterogeneities that impact water, solute partitioning and solubility, and complex water-mediated interactions.

Biography:

Prof. M. Scott Shell is the Myers Founders Chair Professor and Vice Chair of Chemical Engineering at the University of California Santa Barbara. He earned his B.S. in Chemical Engineering at Carnegie Mellon in 2000 and his Ph.D. in Chemical Engineering from Princeton in 2005, followed by a postdoc in the Department of Pharmaceutical Chemistry at UC San Francisco from 2005-07. Prof. Shell's group develops novel molecular simulation, multiscale modeling, and statistical thermodynamic approaches to address problems in contemporary biophysics and soft condensed matter. Recent areas of interest include self-assembled peptide materials, nanobubbles, hydrophobic interfaces, water purification membranes, colloid-polymer materials. He is the recipient of a Dreyfus Foundation New Faculty Award (2007), an NSF CAREER Award (2009), a Hellman Family Faculty Fellowship (2010), a Northrop-Grumman Teaching Award (2011), a Sloan Research Fellowship (2012), a UCSB Academic Senate Distinguished Teaching Award (2014), the Dudley A. Saville Lectureship at Princeton (2015), and the CoMSEF Impact Award from AIChE (2017).

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