Predictive Modeling of Dielectric Effects in Materials

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Abstract

Efficient computer simulation strategies that offer predictive capabilities play a crucial role in the design of new materials. A frequently overlooked factor in this type of modeling, in particular for polymeric and colloidal systems, is the role of dielectric effects. New computational developments have now made it possible to incorporate these effects in predicting self-assembled structures as well as ionic charge transport. I will illustrate the methods that provide these capabilities. Moreover, I will illustrate the consequences of nonuniform permittivity in nanoparticle aggregates as well as ionic transport in confined geometries.

Short Biography

Professor Erik Luijten studied physics in The Netherlands, where he received his MSc from the Institute for Theoretical Physics at Utrecht University and his PhD (cum laude) from Delft University of Technology in 1997. He has worked as a postdoctoral research associate at the Max Planck Institute for Polymer Research and the University of Mainz, Germany, with Prof. Kurt Binder and at the Institute for Physical Science and Technology of the University of Maryland, with Prof. Michael E. Fisher and Prof. Athanassios Panagiotopoulos. From 2001 to 2008 he was an assistant professor and later associate professor in the Department of Materials Science and Engineering and (by courtesy) the Department of Physics at the University of Illinois at Urbana-Champaign. In January 2009 he joined Northwestern University, with appointments in Materials Science and Engineering and Applied Mathematics. As of September 2016, he serves as chair of the Department of Materials Science and Engineering. Professor Luijten received the 2003 IAPWS Helmholtz Award in recognition of "Fundamental and innovative contributions enhancing the state of the art of computer simulations of theoretical models that are directly relevant to the critical and phase behaviour of aqueous systems." He also received an NSF CAREER Award (2004) and a Xerox Award for Faculty Research (2006). In 2013 he was elected Fellow of the American Physical Society.