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Molecular theory of solvation for supramolecular nanostructures and nanomaterials

In recent two decades, molecular theory of solvation for nanostructures in both aqueous and non-aqueous solutions, a.k.a. three-dimensional reference interaction site model (3D-RISM) with the Kovalenko-Hirata (KH) closure relation, was systematically developed and applied to a variety of compounds, supramolecules, and biomolecules in a number of solvents, solvent mixtures, electrolyte and non-electrolyte solutions. From the first principles of statistical mechanics, 3D-RISM-KH theory predicts the solvation structure and thermodynamics of nanochemical and biomolecular systems, including their analytical long-range asymptotics. It yields improved accuracy, efficiency, and applicability by coupling models and methods at different space and time scales to provide fundamental understanding and prediction for nanomaterials and biomolecules. The method has been coupled with quantum chemistry, molecular dynamics, and dissipative particle dynamics. Examples include helical rosette nanotubes with tunable stability and hierarchy, water promoted inversion of supramolecular chirality, formation and stability of self-assembling supramolecular structures of organic rosette nanotubes with ordered shells of inner and outer water, and highly accurate & efficient dissipative particle dynamics of polymer chains with coarse-grained effective pair potential obtained from DRISM-KH theory. Recent applications of 3D-RISM-KH consist in multiscale coupling of quantum chemistry, molecular solvation theory, multi-time step molecular dynamics, and dissipative particle dynamics. Calculations show the dependence of the polymerization degree on organic solvents properties and temperature/pressure change. Aggregation of kaolinite platelets due to face-to-face, edge-to-face, and edge-to-edge interactions and temperature/pressure strongly affect bioadsorption on clays and flocculation of clay nanoparticles in aqueous and non-aqueous solutions with polymers. Multi-Time-Step Molecular Dynamics coupled with 3D-RISM-KH molecular solvation theory and Generalized Solvation Force Extrapolation (MTS-MD/3D-RISM-KH/GSFE) provides quasidynamics description of biomolecules. Validation included folding of miniprotein in solution from fully extended to equilibrated state in 60 ns, which provides acceleration by two orders of magnitude time scale as compared to 4-9 μs protein folding in experiment.

Biography

Andriy Kovalenko is Senior Research Officer at the National Institute for Nanotechnology since 2003, and Adjunct Professor in the Department of Mechanical Engineering at the University of Alberta, Edmonton, Canada. He earned his PhD degree (1993) in Theoretical and Mathematical Physics from Lviv State University, Bogolyubov's Institute. He has been developing methodology and software implementation of statistical-mechanical, molecular theory of solvation, coupling it with electronic structure theories, molecular simulations, and docking protocols in a platform of predictive multiscale theory & modeling of chemical, supramolecular, and biomolecular systems constituting new advances towards a general framework of multiscale methods.

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