Molecular theory of solvation and its application to chemical and biomolecular systems and nanobiomaterials

Visiting professor: Andriy Kovalenko (University of Alberta, Cananda)

Course description:

These lectures will introduce the methodology of the 3D-RISM-KH molecular theory of solvation and illustrate its predictive capabilities for various chemical species and nanoparticles in different solvents and liquid mixtures, electrolyte solutions, self-assembling supramolecular nanoarchitectures, biomolecular systems, and nanobiomaterials. Based on the first principles of statistical mechanics, the 3D-RISM-KH theory bridges the gap between molecular structure and effective forces and processes occurring in nanosystems in solution at long time scales. It is uniquely capable of predicting chemistry-driven effective interactions in chemical and biomolecular systems. The 3D-RISM-KH theory yields the solvation structure and thermodynamics from classical interaction potentials specified with a molecular force field and thus links molecular structure to the macroscopic world of thermodynamic observables and effective colloidal interactions.

Syllabus of the lecture subjects (enlisted):

1. Statistical thermodynamics of solvation
2. Integral equation theory of molecular liquids and solutions
3. Solvation thermodynamics of chemical compounds
4. Partitioning between different solvents
5. Prediction of structural water in biomolecular systems
6. Molecular recognition and protein-ligand binding
7. Protein-protein effective interactions in solution, including aggregation, oligomers and fibrils formation
8. Self-assembly, conformational stability, transitions and functions of synthetic organic supramolecular nanoarchitectures (organic rosette nanotubes)
9. Nanoscale forces that control plant cell wall recalcitrance; towards integrated process of biomass conversion to second generation biofuels and bionanomaterials
10. Effective interactions and properties of modified cellulose nanocrystals (CNC) for industrial applications

Projekt „Rozwój interdyscyplinarnych studiów doktoranckich na Politechnice Gdańskiej w zakresie nowoczesnych technologii” jest współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego.

TERMINY ZAJĘĆ			
Data	**Dzień tyg.**	**Godz.**	**Sala**
2015-06-08	poniedziałek	12.00-15.00	Luwr (Chemia A)
2015-06-09	wtorek	12.00-15.00	Luwr (Chemia A)
2015-06-10	środa	12.00-15.00	Luwr (Chemia A)
2015-06-11	czwartek	12.00-15.00	Luwr (Chemia A)
2015-06-12	piątek	12.00-15.00	Luwr (Chemia A)

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