Applied Molecular Modeling (CHEM 512, call # 30748)

Elective 3-credit course for graduate students of:

all Specializations in **Chemistry** (physical, analytical, organic, inorganic), **Chemical Biology**, **Nanoscience**,
also available to students of Physics, Medicinal Chemistry, Bio-sciences, and Engineering

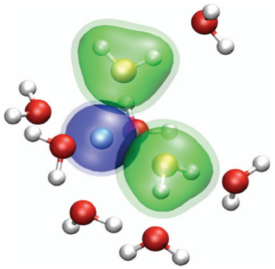
Prerequisites: **graduate students:** none, undergrads: consent by instructor (Prof. D. Bratko, https://chemistry.vcu.edu/people/faculty/bratko.html). Jan 14-May 3, 2019, TR 12:30-1:45, Temple 2226

Would you like to learn *the principles behind molecular simulations*?

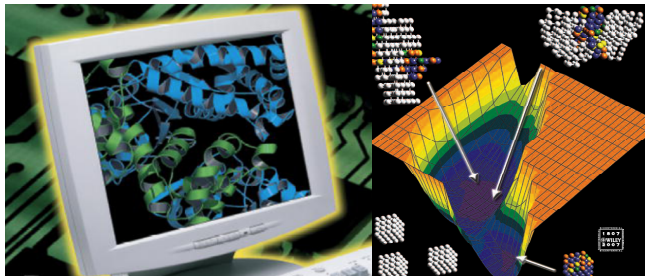
What are their strengths and weaknesses, and how can they advance *your* research?

Through seminars and *hands on study-cases*, this course will prepare you for informed and creative usage of simulation tools in:

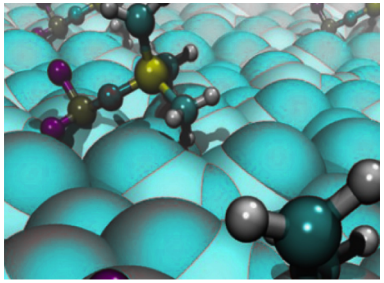
Chemistry and Molecular Physics,



Chemical Biology and Biophysics



Materials and Nanomaterials



and more! You will learn how to design or modify your code, and take advantage of continued progress in the field. For more information, see the attached Syllabus or contact the instructor (dbratko@vcu.edu, Oliver Hall Physical Sciences 4021, 828-1865).

Applied Molecular Modeling (CHEM 512) Syllabus

Graduate Course, 3 credits

Outline: Aimed at students of chemistry, engineering, (bio)physical and nanosciences with research interests in *molecular and mesoscopic* modeling involving computer simulations:

- Molecular models; Molecular Dynamics and Monte Carlo approaches, visualization.
- Seminars and hands-on experience in *designing*, customizing and use of programs to study molecular fluids, biomolecules, and nanoparticles.
- Introduce the student to simulation techniques *for his or her research* ranging from chemical thermodynamics, solutions and polymers to surface chemistry and catalysis.

Recommended background: Thermodynamics with elements of statistical thermodynamics (CHEM 303 or PHYS 340 or CHEM 511 or CHEM 612). Essentials of ensemble statistics, programming and Linux operations will be covered as necessary.

Topics:

Model systems: molecular force fields and coarse-grained representations
Computer simulations: purpose/motivation, modeling of small systems, connection with thermodynamics and statistical mechanics
Monte Carlo methods: importance sampling, Metropolis method, monatomic fluids, complex molecules
Molecular Dynamics: equations of motion, force calculations, integration schemes, polyatomic molecules, Brownian dynamics
Ensembles: canonical (N,V,T), microcanonical (N,V,E), isothermal-isobaric (P,V,T), grand canonical ensemble (μ,V,T)
Phase equilibria: Free energy and chemical potential calculations, Gibbs ensemble, semi-grand ensemble, applications
***Advanced techniques*:** methods of constraints, long-ranged interactions, polymer modeling, anisotropic systems, rare events
Computational efficiency, programming

Principal text: D. Frenkel and B. Smit, Understanding molecular simulation. From algorithms to applications, Academic, 2002.
Supplementary: M. P. Allen and D. J. Tildesley, Computer Simulation of Liquids, Oxford University Press, 2017.

Requirements: active participation, completion of weekly homeworks and study-cases, a term paper and seminar presentation