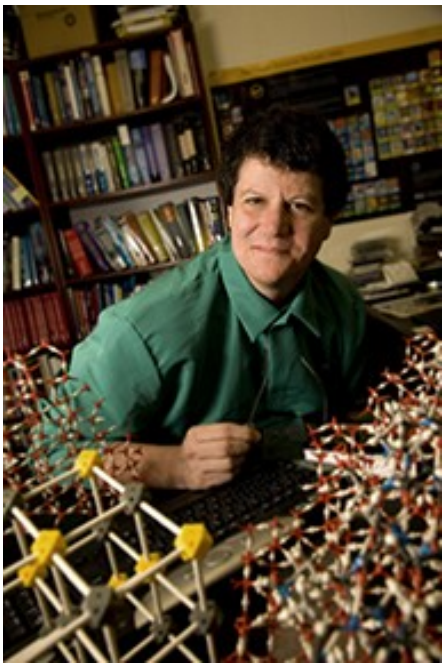
John P. McGovern Lectureship in Biomedical Computing and Imaging

Simulations of Biomolecules in Solution and Bilayers



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The ability to simulate the dynamics of proteins has been around for more than thirty years. Initial simulations of proteins were in the gas phase and only for a few picoseconds. Yet these simulations provided insight into the structure, function and dynamics of proteins. With advances in theory, software, and computer hardware we are able to perform long simulations on the order of 100s of nanoseconds that include solvent, salt, and lipid bilayers. We have recently focused our computational efforts on two problems. The first effort is the impact salt play in the stability of short (~21 amino acid) peptides. The second effort is in the area of transporters specifically leucine, dopamine and serotonin. In this talk I will present some of our recent finding on these topics.

Date: Wednesday, January 6, 2010
Time: 4:00PM
Place: GSBS Large Classroom (BSRB S3.8371)
Mitchell Basic Sciences Research Building
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