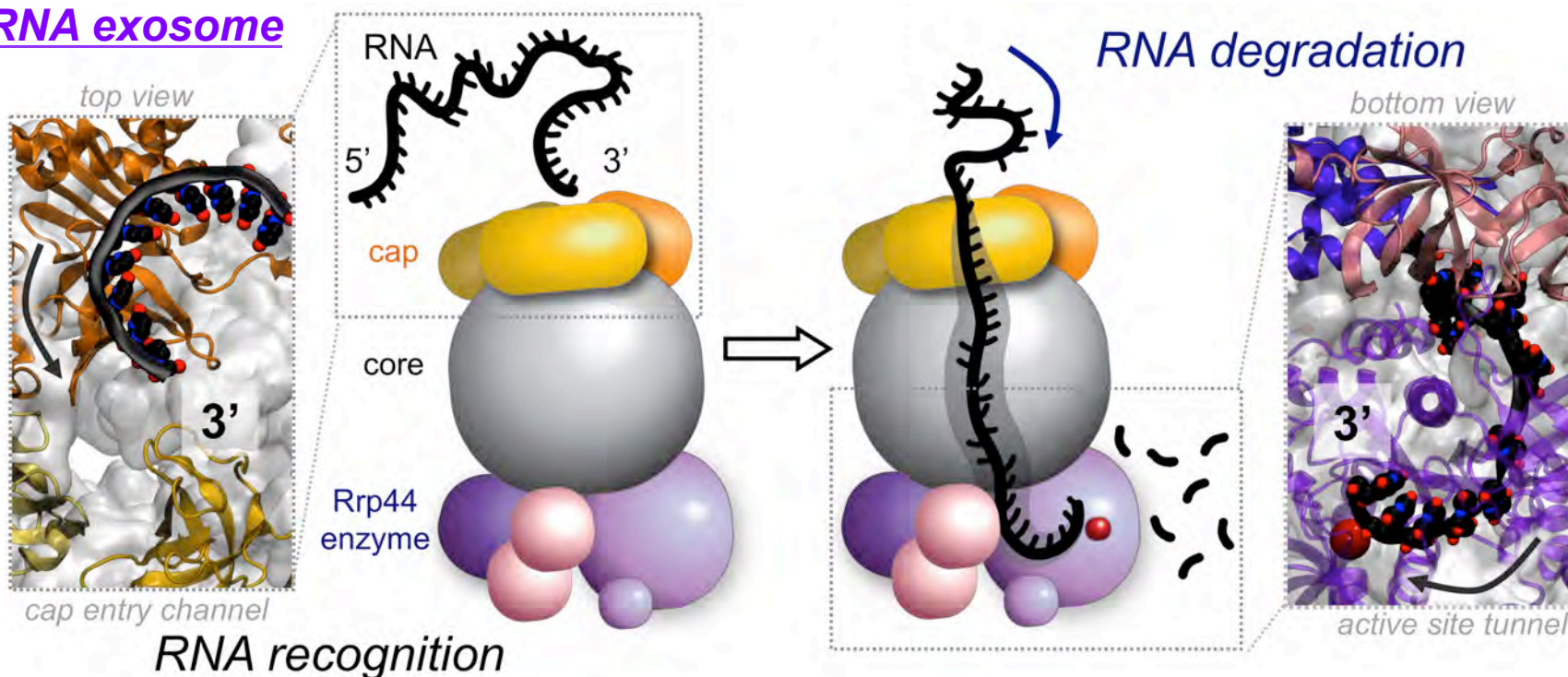
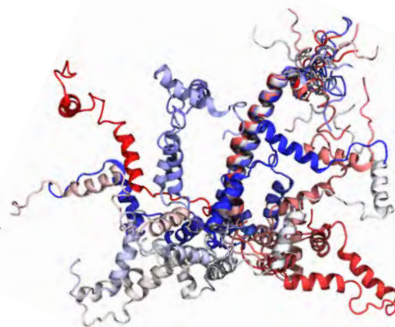


Functional mechanisms of biomolecules: *cellular quality control machinery*RNA exosome**New methods for biomolecular simulations**

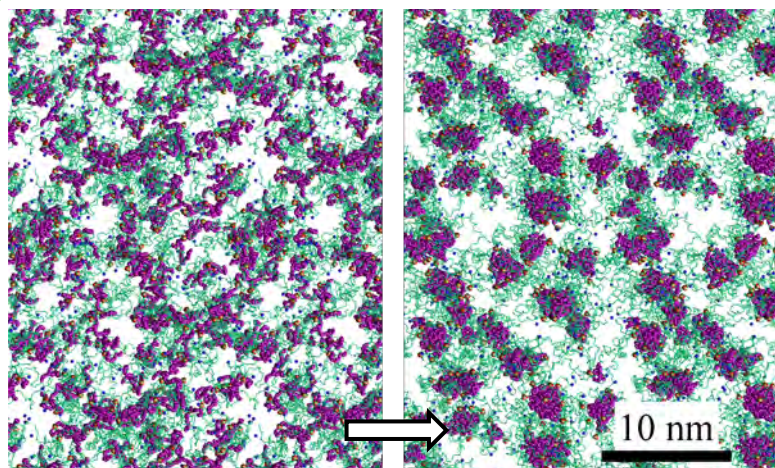
New techniques are required to describe functional motion of biomolecules, which occurs on long timescales. We plan to develop new **coarse-grained representations** of biomolecules and new enhanced sampling techniques.



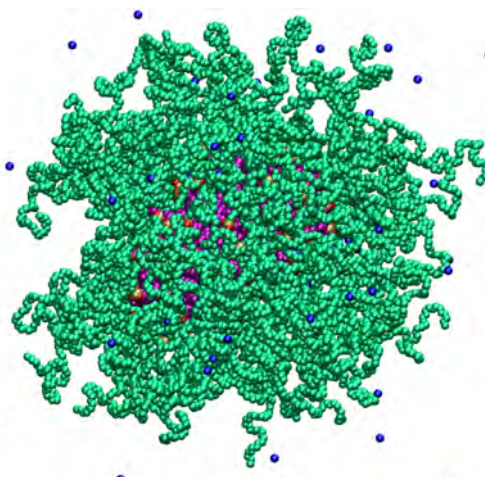
We are looking for new undergraduate and graduate students with chemistry, physics, or programming background. If interested, please contact Lela at: **Lvukov1@gmail.com**

... starting Jan 2016 ...

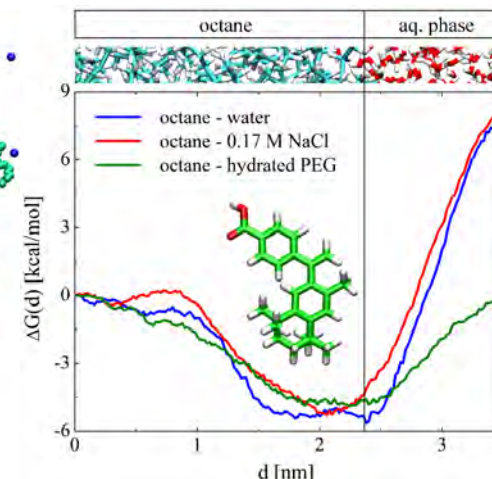
Functional material nanoassemblies



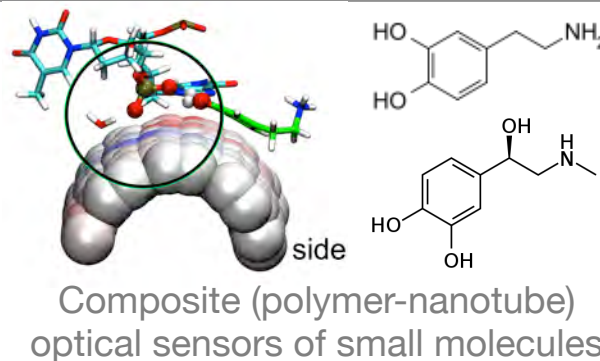
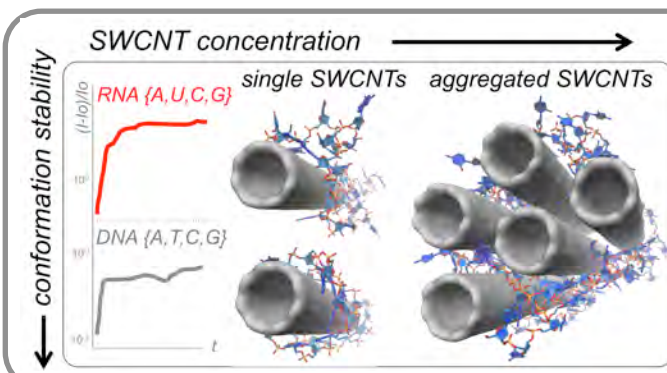
Polymer self-assembly



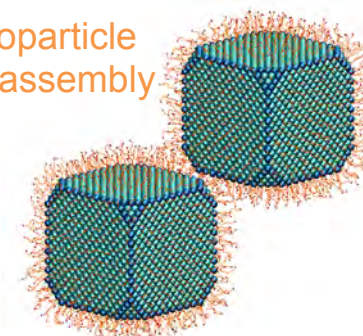
Drug-delivery nanocarriers



Drug solvation properties



Nanoparticle self-assembly



Research in our theory group is devoted to modeling of realistic biological and materials systems in close collaboration with experimentalists. We use quantum and classical molecular dynamics simulations, and other advanced computational techniques to study: 1) biomolecular complexes, primarily involved in cellular quality control; 2) self-assembled polymeric and composite nanomaterials with important functionalities. The calculations will be performed on our multiprocessor and GPU clusters and on national supercomputers.