

Available software

We are expanding the software on the cluster. Currently, the following software is available for scientific computing and visualization:

Fortran 90, C++

NAMD2.6

NAMD 2.7b2 (GPU acceleration)

VMD1.8.6

GROMACS 3.3.3

GAUSSIAN3.0

GAUSSVIEW

SIESTA3.0-b

We plan to add soon VASP and the GPU version of GROMACS

Prof. Petr Král's group is also developing hybrid software which will allow to perform simultaneous ab-initio quantum transport calculations and molecular dynamics simulations (funded proposal: NSF-CBET 0932812).

** If you need to run some specific software which is not listed above please contact the administrator

Become a cluster user

Usage policies:

1. UIC Chemistry Department faculty, staff, postdocs, and students, please contact Ms. Lela Vuković to obtain an account.
2. There is no limit on the character of calculations performed and quota limit on the disk space usage, however, the overall cluster usage is monitored.
3. It is the users responsibility to run the calculations effectively and keep their data securely stored elsewhere. For initial advising, please contact Ms. Vuković.

Account Request:

To get an account, please send an email to lvukov1@uic.edu with these details:

1. What is your full name?
2. What group are you in?
3. What is your office room number?
4. What is your office telephone number and UIC email address?
5. What would you like for a login ID? (Maximum length is 10 characters)

Student Training

New users can receive initial training in:

- using Linux operating systems
- using Gaussian and NAMD computational software
- using Gaussview and VMD visualization software
- running calculations on GPUs
- setting up connections from the cluster to the lab desktops/laptops

Linux help: <http://unixhelp.ed.ac.uk/index.html>

Additional training can be obtained in the Chem 402 course:
Chemical Information Systems

Consulting

Buying new computer hardware?

If your group plans on buying a new computer, we may recommend specific components and models, appropriate to the planned use

Applying for external computation time

Individual research groups can apply for computation time on UIC cluster and for allocations on external resources:

1) UIC high performance computing on the ACCC Cluster Argo

<http://www.uic.edu/depts/accc/hardware/argo/index.html>

2) These and other supercomputer resources are also available:

National Supercomputing Centers (NCSA)

<http://www.ncsa.illinois.edu/>

National Energy Research Scientific Computing Center (NERSC)

<http://www.nersc.gov/>

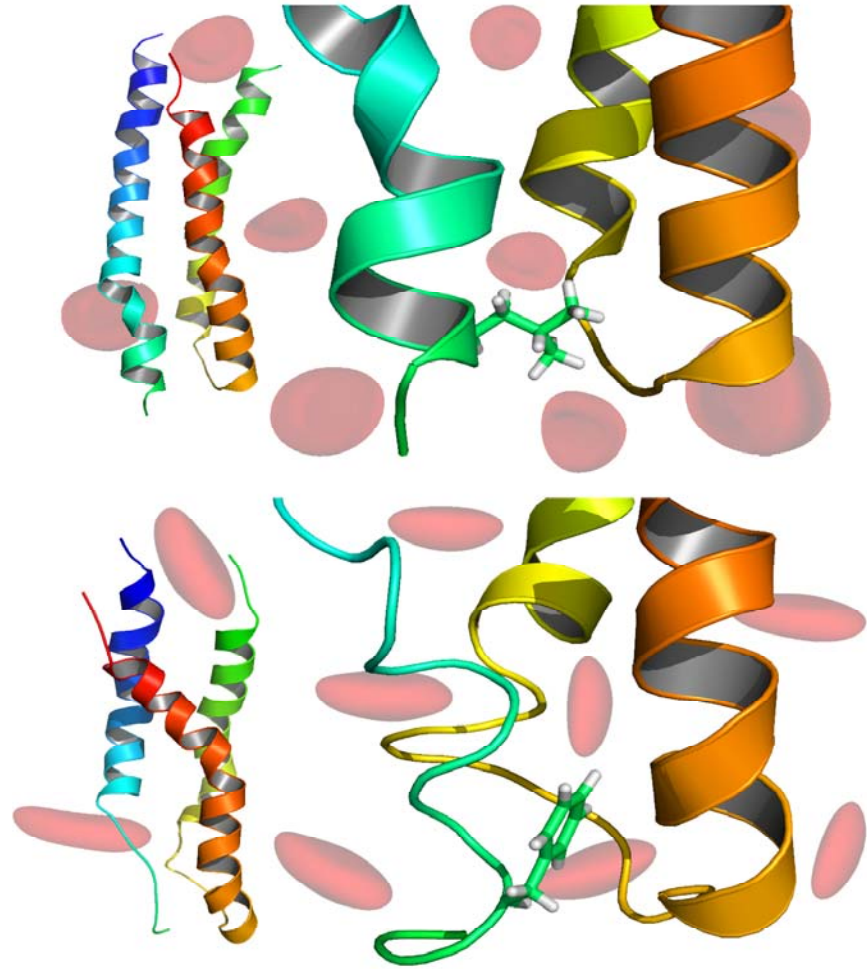
Center for Nanoscale Materials (CNM)

<http://nano.anl.gov/>

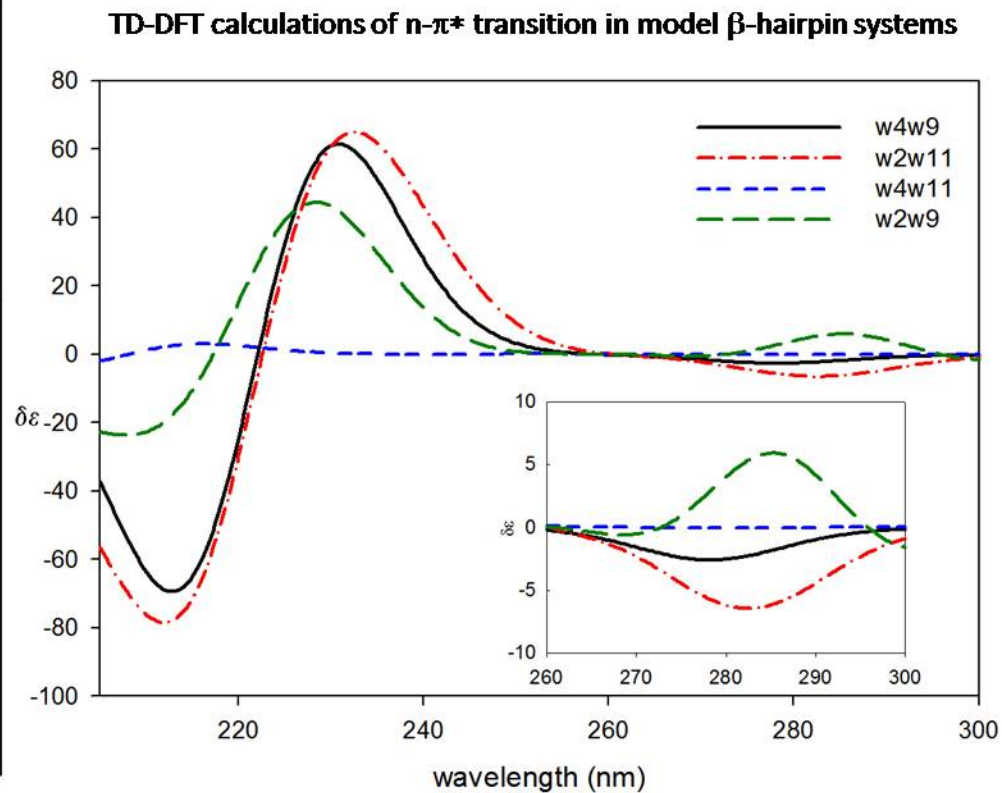
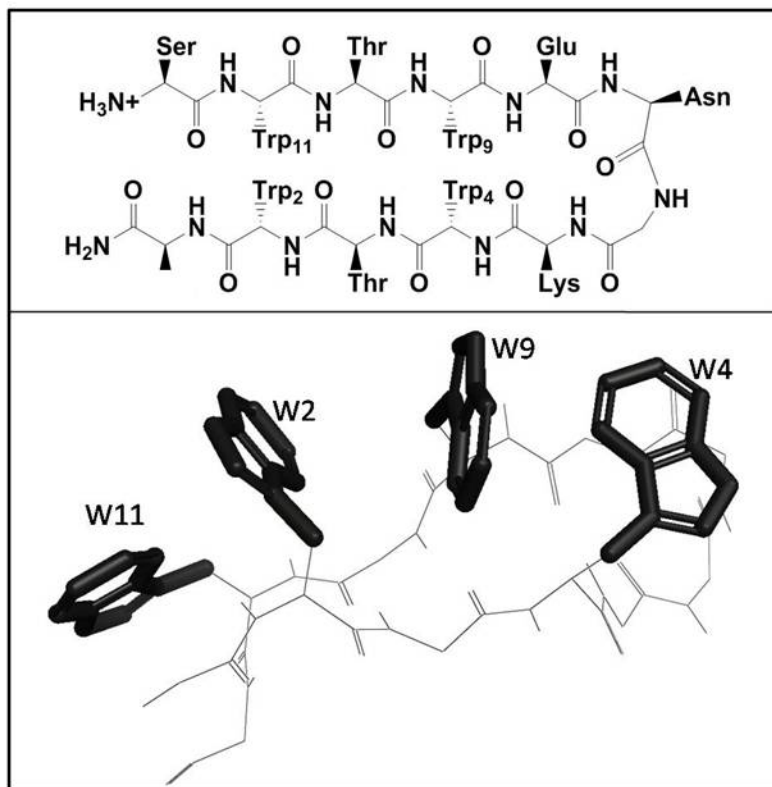
Picture Gallery

Prof. Fung's group

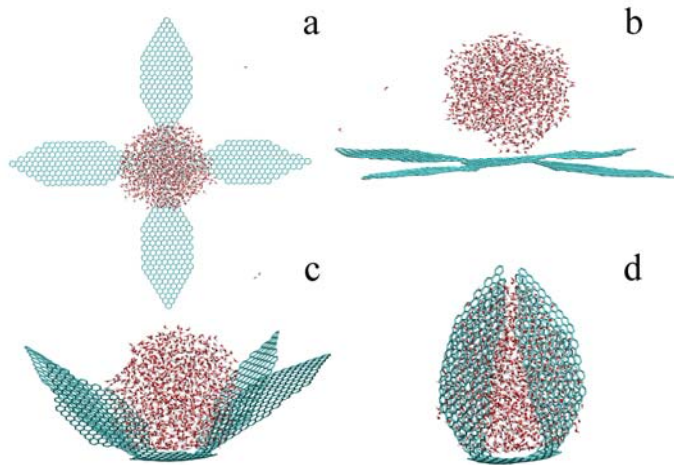
Normal (top) and abnormal (bottom) complex of erythroid alpha-spectrin and beta-spectrin helices, obtained from homology modeling and molecular dynamics simulations. Overlaid are corresponding erythrocytes, simulated with simple geometric functions.



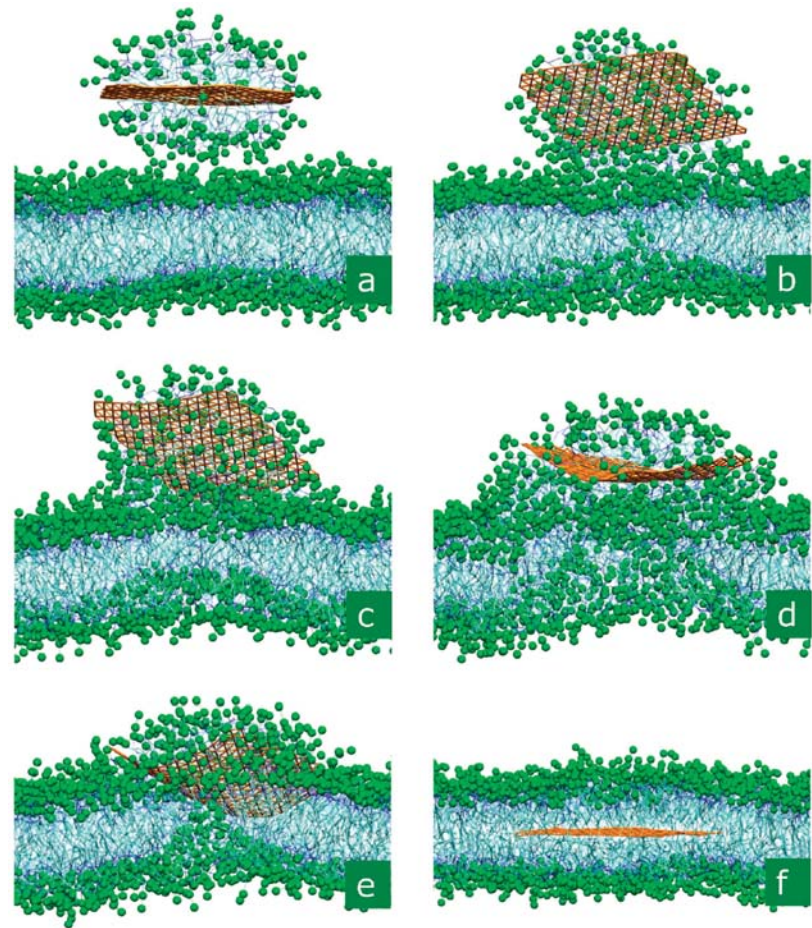
Prof. Keiderling's group



Prof. Král's group



Nanodroplet-assisted folding of a star-shaped graphene flake



Insertion of graphene into phospholipid membrane

Contact Information:

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