# Computational Modeling Core Mini-symposium

**Date: Wednesday May 2nd**
**Location: University of Chicago, Gordon Center for Integrative Science (GCIS), room W301**

## Schedule:

**8:00 AM Breakfast and welcome**

**AIM 1**

8:30 — Lei Huang — Webserver for automated optimization force field parameters

8:50 — Christopher Mayne — VMD interface and automated force field optimization

9:10 — Wei Han — Development of a multiscale CG model for protein folding, aggregation and dynamics in membrane

9:30 — Emad Tajkhorshid — Developing an atomistic, highly mobile membrane model (HMMM) and its wide applications

9:50 — Fatemeh Khalili — Asymmetric membrane potential and ionic concentration

10:10 — Janamejaya Chowdhary — polarizable force field for lipid membranes

**AIM 2**

10:30 — Shahid Islam — KcsA modeling with spin label distribution from ESR/DEER histogram distances

10:50 — Fatemeh Khalili — Na/K Pump probed by LRET

11:10 — Elia Zomot — The crystallized structure of the carnitine/γ—butyrobetaine antiporter CaiT is a substrate-releasing conformation

11:30 — Hang Yu — Membrane Sculpting by F-BAR Domains studied by Molecular Dynamics Simulations

**Break for lunch**

**AIM 3**

12:30 PM — Avisek Das — Conformational transition pathways from coarse grained ANM normal modes

12:50 — Mert Gur — Transition pathways of dopamine transporters explored by combining molecular dynamics simulations and monte carlo sampling of collective modes

1:10 — Mahmoud Moradi — Optimizing Transition Pathway for Large—Scale Conformational Changes in ABC Transporters Using Non—Equilibrium Work

1:30 — Giray Enkavi — Chemomechanical Coupling in MFS Transporters

1:50 — Wei Han — Proton Transfer Pathway in CIC Antiporter

**AIM 4**

2:15 — Wonpil Im — restrained ensemble for solid state NMR (special talk of 30 min)

**Emad Tajkhorshid Group** **Klaus Schulten Group** **Ivet Bahar group** **Benoit Roux Group**