

# RISE OF the machines™

Integration of experiment, simulation and theory for a mechanistic understanding  
of biomolecular machines

Organizers: Ioan Andricioaei, Sichun Yang and Jingzhi Pu

Telluride Intermediate School @ 725 W. Colorado

Aug. 5-9, 2013

TSRC Hosts: Exec Director, Nana Naisbitt (970-708-0004)

Asst Director, Rory Sullivan (970-708-0004)

“Molecular machines” such as bio-molecular motors and ion pumps are fascinating subjects for study because they transform energy between different forms in an efficient manner. The functional mechanism of molecules machines is often complex and involves numerous physical and chemical processes that occur at multiple spatial & temporal scales. Therefore, it is increasingly clear that the most productive strategy would be to integrate experiment, molecular simulation and theory. In reality, however, such integration is rarely done and the three disciplines remain largely segregated. In this workshop, we bring together active investigators in these three disciplines to identify and discuss burning mechanistic questions concerning molecular machines that will best benefit from an effective integration of experiment, simulation and theory. In addition to discussions of recent technical developments, specific mechanistic findings and novel ideas/hypotheses, we hope the workshop can help reduce communication barriers between different disciplines and foster new collaborations.

## Aug. 4<sup>th</sup> Sunday

6:00 – 8:00pm: Informal gathering at the New Sheridan Bar (231 W. Colorado) for drink specials and free pool. A TSRC employee will be there to greet people and answer questions.

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**Total: 4+5+4+4=17**

## Aug. 5<sup>th</sup> Monday [4]

8:15am Breakfast at Telluride Intermediate School, 2<sup>nd</sup> Floor  
**Registration, 1<sup>st</sup> Floor**

8:45am Meeting at Telluride Intermediate School, 2<sup>nd</sup> Floor

8:45-9:00am Introduction, organizers/Nana Naisbitt, TSRC director

9:00am Jingzhi Pu (IUPUI) “Simulating ABC-transporters using a multiscale approach”

9:45am Ruxandra Dima (Cincinnati) “Exploring the mechanical action of molecular motors during the depolymerization of cytoskeletal filaments”

**10:30 am Coffee Break**

10:45am George Stan (Cincinnati) “Computational studies of protein unfolding and translocation through repetitive pulling in allosteric cycles of AAA+ motors”

11:30am Arvind Ramanathan (Oak Ridge) “Elucidating the structure of disordered proteins by integrating neutron scattering, atomistic simulations and statistical inference”

**Aug. 6<sup>th</sup> Tuesday [5]**

8:15am Breakfast Telluride Intermediate School, 2<sup>nd</sup> floor

8:45am Meeting at Telluride Intermediate School, 2<sup>nd</sup> floor

8:45am Ronald Hills (New England) “Modeling conformation and bilayer dynamics in the ABC transport cycle”

9:30am Robert Jernigan (Iowa State) “How limited are the motions of large bio-machines and do these motions always relate to function”

**10:15am Coffee Break**

10:30am Ron Dror (Shaw group) “How drugs bind and control their targets: characterizing GPCR signaling through atomic-level simulation”

11:15am Gianluigi Veglia (Minnesota) “Regulation of Ca<sup>2+</sup>ATPase function by phospholamban conformational equilibrium”

12:00am Ioan Andricioaei (UC Irvine) “Simulations of supercoil removal by topoisomerases and viral DNA ejection/import”

**6:00pm Town Talks @ Historic Sheridan Opera House at 110 N. Oak**

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**Aug. 7<sup>th</sup> Wednesday [4]**

8:30am Breakfast Telluride Intermediate School, 2<sup>nd</sup> floor

8:45am Meeting at Telluride Intermediate School, 2<sup>nd</sup> floor

8:45am Wenjun Zheng (Buffalo) “Recent development in coarse-grained modeling and all-atom simulation of protein structures and dynamics”

9:30am Lee Makowski (Northeastern) “Correlation of small-angle x-ray solution scattering with MD trajectories: Common measures, different time-scale”

- 10:15am**      **Coffee Break**
- 10:30am      Barry Grant (Michigan) “Dynamic coupling in molecular switch and motors”
- 11:15pm      Alessandro Cembran (Minnesota) “Computer simulations of protein kinase A”
- 6:00pm**      **Picnic @ Ah Haa School for the Arts at 300 S. Townsend**
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**Aug. 8<sup>th</sup> Thursday [4]**

- 8:30am      Breakfast Telluride Intermediate School, 2<sup>nd</sup> floor
- 8:45am      Meeting at Telluride Intermediate School, 2<sup>nd</sup> floor
- 8:45am      Sichun Yang (Case Western Reserve) “Coarse-grained simulations of protein-protein assembly”
- 9:30am      Andrzej Kloczkowski (Ohio State) “Normal mode analysis for quantitative understanding of the dynamics and proteins and biomolecular machines”
- 10:15am**      **Coffee Break**
- 10:30am      Yinghao Wu (Albert Einstein) “Multiscale modeling of cadherin-mediated cell adhesion”
- 11:15am      Fangqiang Zhu (IUPUI) “Calculating ion channel conductance from all-atom simulations”
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**Aug. 9<sup>th</sup> Friday [0]**

- 8:30am**      **Breakfast and Wrap-up Session**