

**Introduction to Molecular Dynamics and OpenMM Zephyr Workshop
Clark Center Room S361**

Friday, June 26, 2009

9:00am – 9:10am	Welcome and introduction of instructors and workshop attendees - <i>Vijay Pande</i>
9:10am – 10:10am	Introduction to molecular dynamics - <i>Vijay Pande</i>
10:10am – 11:00am	Introduction to OpenMM Zephyr - <i>You, with guidance from Joy Ku</i>
11:00am – 12:30pm	LUNCH (on your own)
12:30pm – 1:15pm	Exploring more OpenMM Zephyr features - <i>You, with guidance from Joy Ku</i>
1:15pm–2:15pm	Introduction to advanced topics in molecular dynamics - <i>Vijay Pande</i>
2:15 pm – 2:30pm	BREAK
2:30pm – 3:30pm	Exercise: Using OpenMM/mdrun to run simulations with additional parameter settings - <i>You, with guidance from Mark Friedrichs</i>
3:30pm – 4:45pm	Break-out Sessions: Use OpenMM Zephyr and OpenMM/mdrun to answer your research question
4:45pm – 5:00pm	Wrap up and Q & A - <i>All</i>