Chemical & Physical Sciences
UNIVERSITY OF TORONTO
MISSISSAUGA

COLLOQUIUM

TUESDAY OCTOBER 18TH, 2011
12:00 P.M. – 1:00 P.M.
COUNCIL CHAMBERS (DV 3130)

Martin Gruebele

University of Illinois at Urbana-Champaign

"Fast protein folding: finally feedback between computation and experiment."

Protein folding is at the verge of an era not unlike small molecule structure and dynamics 20 years ago, when quantum chemistry calculations crossed a threshold of ease and reliability. I will discuss how speeding up experiments into the microsecond regime, and lengthening molecular dynamics simulations into the millisecond regime, finally has brought the two together in a way that is improving our ability to predict how proteins fold "ab initio." Experiments on several model proteins will be compared with calculations, and the progress from predicting roughly folded states just ten years ago, to X-ray accuracy computed structures and experimentally verified computed mechanisms and kinetics will be charted.