



The Abdus Salam
**International Centre
for Theoretical Physics**



**College on Multiscale Computational Modeling of
Materials for Energy Applications
4 - 15 July 2016**

Co-sponsors: INRS Canada, ESF and Psi-k

Classical Molecular Dynamics for Nanosystems: LODiS Software"

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Abstract:

After a review of molecular dynamics algorithms -including metadynamics-, we will discuss the peculiarity of nanosystems and how we can model them. A lab to practice with LoDiS-MD software (low dimensional system molecular dynamics) will follow. Melting and freezing transitions, example of growth models will be considered as examples.