# CH247 Jan 3:0

# Introduction to molecular simulations

## Instructor

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## Teaching Assistant

Email:

**Department: Chemical Engineering**

Course Time:

Lecture venue: Chemical Engineering Class Room

Detailed Course Page:

## Announcements

## Brief description of the course

The course teaches a student to perform molecular dynamics and Monte Carlo molecular simulations. The course covers both basic as well as advance algorithms in molecular simulations. Students will also learn to write their own molecular simulation code.

## Prerequisites

Any Graduate Thermodynamics course

## Syllabus

Introduction to molecular dynamics; conservation laws; integration schemes: verlet, velocity verlet, leap-frog; constraint dynamics; extended Lagrangian dynamics; Thermostats and barostats; introduction to Monte Carlo techniques; Metropolis algorithm; NVT, NPT and GCMC simulations; estimation of pressure, chemical potential, radial distribution function, auto-correlation function, Ewald summation; umbrella sampling; Gibbs Ensemble technique; configuration bias technique.

## Course outcomes

The student will learn both basic and advanced molecular simulation techniques. Also upon successful

completion, the student will be able to write his/her own code for performing molecular simulations.

## Grading policy

50% for assignments, 50% for project

## Assignments

## Resources

M. P. Allen and D. J. Tildesley, Computer simulation of Liquids, Oxford University Press, New York, 1987

D. Frenkel and B. Smit, Understanding Molecular Simulation: From Algorithms to Applications, 2nd Ed., Academic Press, San Diego, 2002