Advanced Computational Physics

Riccardo Ferrando, Diana Nelli (Univ. Genova)

• *The energy landscape: properties and complexity (R. Ferrando)*
- Funnel-like and glassy potential energy surfaces
- Inherent structure
- Calculating the partition function: superposition appoximation
- Transition rates: Transition State Theory, Kramers Theory

• *Exploring the energy landscape: energy minima (R. Ferrando, D. Nelli)*
- Basics of Monte-Carlo and Molecular Dynamics simulations
- Global optimization
- Basin Hopping algorithm
- Genetic algorithms

• *Exploring the energy landscape: looking for saddle points (R. Ferrando)*
- Nudged Elastic Band method
- Eigenvector Following

• *The free-energy landscape (D. Nelli)*
- Collective variables
- Metadynamics

• *Applications (D. Nelli)*
- An introduction to metallic nanoparticles
- Global optimization of nanoparticles
- Structural transformations and phase transitions in nanoparticles