Microscopic simulations of condensed states

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Modulo a scelta da 2 CFU per studenti del corso magistrale di Fisica, del corso magistrale di Chimica e Materiali, e del dottorato di Fisica e Chimica. Il corso prevedere circa 16 ore di lezioni frontali da svolgersi a partire dalla metà di novembre con modalità ed orari da concordare tra il docente e gli studenti interessati. Per esprimere il proprio interesse al corso e per eventuali altre informazioni rivolgersi al Prof. Carlo Pierleoni (carlo.pierleoni@aquila.infn.it).

Syllabus

1. Equilibrium Thermodynamics and Statistical Mechanics framework (essentials). Ensembles, thermodynamic potentials, thermodynamic properties.
2. Modelling solid and liquids:
   (a) Intermolecular and Intramolecular potentials: the effective model approach (Hard cores, Lennard-Jones, point charges, etc.).
   (b) Periodic boundary conditions versus effective substrate external fields.
3. Statistical Mechanics expressions of relevant thermodynamic and structural properties for the specific simulation models: pressure, reduced distributions, order parameters, etc.
4. Molecular Dynamics: Time correlation functions and transport properties (diffusions, viscosities, thermal conductivity)
5. Monte-Carlo (Metropolis): Method and applications. Phase diagram of the LJ system.
6. Free energy methods: thermodynamic integration, Frenkel-Ladd Einstein crystal method.
7. Phase diagram of bulk liquid crystals: the isotropic-nematic transition.
8. Phase diagram of polymer melts and polymer solutions (good solvent, theta solvent): random walk model-SAW model- Monte-Carlo calculations on lattices and in continuous space.

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