1) Description of Molecular Dynamics

2) The basic concepts
   - Modeling a physical system
     Example: Lennard-Jones potential
   - Periodic boundary conditions
   - Time integration algorithm
     Verlet algorithm, predictor-corrector algorithm

3) Running, measuring, analyzing
   - Starting a simulation, controlling the system, equilibration
   - Simple statistical quantities to measure potential energy, kinetic energy, total energy, temperature

4) Simulating in different ensembles
   - microcanonical, canonical, macrocanonical

5) Examples of interatomic potentials
   - application to two-body potentials

**Literature**

**Articles**