

PROJECTS
Computational Nanoscience
SoSe 2016 (66-990)
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Erforderliche Vorkenntnisse: Kursvorlesungen Quantenmechanik

Inhalt – mögliche Themen:

1. Numerical Solution of non-linear oscillator
2. Classical Molecular Dynamics with Verlet algorithm
3. Solution of Time-dependent Schrödinger Equation
4. Variational Method in Quantum Mechanics: Secular Equation
5. Hartree-Fock Method for Nanosystems
6. Density-Functional Calculations for Nanosystems
7. Tight-Binding Model for Graphene
8. Quantum Nanosystems: Exact-Diagonalization
9. Monte Carlo scheme for Ising Nanomagnets
10. Quantum Monte-Carlo for Heisenberg Model
12. Numerical Solution of Schrödinger Equation for Nanosystem
13. Electronic structure of Nanosystems
14. Computational Nanoscience: Molecular Dynamics
15. Computational Nanoscience: DFT for real system