Ab initio molecular dynamics: basic theory and advanced methods

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Tuesday **8.30 (ST)-10.00;** Seminarraum E **Bau 2/413, 01-231**

Begin: Tuesday 29. October 2013

Ab initio molecular dynamics has revolutioned the field of computer simulation of complex molecular systems and processes, allowing the description of chemical reactions and unifying molecular dynamics and electronic structure theory.
In this course we present an overview of methods and their application, from basic theory to more advanced methods.

Topics covered in the course include:

- **Basic Techniques**: unifying MD and electronic structure:
  Born-Oppenheimer MD, Car-Parrinello MD and Ehrenfest MD.
  plane wave implementation and pseudopotentials
  thermostats and barostats

- **beyond standard ab initio MD:**
  ROKS, surface hopping and time-dependent DFT

- **Properties from ab initio simulations:**
  vibrational spectroscopy; redox properties

- **Free energy calculations:**
  Free energy perturbation theory
  the blue moon ensemble approach
  umbrella sampling
  metadynamics

- **Response functions and transport coefficients:** Green-Kubo and NEMD

- **The Feymann Path integral**

If you are interested to come, but you cannot come on the first lecture, please send us an e-mail, so I can have an estimate of the numbers. For **more informations** please contact us at
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