Freie Universität Berlin

Institut für Chemie und Biochemie
PD Dr. Dirk Andrae
☎ (030) 838 53757
E-Mail: dirk.andrae@fu-berlin.de

Announcement of a lecture (21358a, 2 hrs / week) with exercises (21358b, 3 hrs / week)

Quantum Reaction Dynamics

Topics:

- **Time-dependent Schrödinger equation**
- **Wavepacket dynamics**
- **Interaction between matter and light**
- **Born-Oppenheimer approximation and beyond**
- **Pump-probe spectroscopy**
- **Wavepacket interferometry**
- **Laser control of chemical reactions**
- **Numerical methods**

Dates and times:

Lectures (starting 17-Apr-2012)
every Tuesday, 08h30 – 10h00, SR 24.16, Takustr. 3

Tutorial (starting 23-Apr-2012)
every Monday, 09h00 – 10h00, SR 24.16, Takustr. 3

Computer Lab (starting 20-Apr-2012)
every Friday, 10h00 – 12h00, PC pool, Chemistry Library, Takustr. 3

- Credit points: 6 (Master Programme in Chemistry).
- The lecture and the tutorials will be in English.

For more information see `http://userpage.chemie.fu-berlin.de/~andrae`

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Quantum Reaction Dynamics
Overview of the time schedule in the Summer Term 2012

Tue, 17-Apr-2012	—	Lecture
Fri, 20-Apr-2012	—	Computer Lab
Mon, 23-Apr-2012	—	Tutorial
Tue, 24-Apr-2012	—	Lecture
Fri, 27-Apr-2012	—	Computer Lab
Mon, 30-Apr-2012	—	Tutorial
Tue, 01-May-2012	—	**No lecture** (public holiday)
Fri, 04-May-2012	—	Computer Lab
Mon, 07-May-2012	—	Tutorial
Tue, 08-May-2012	—	Lecture
Fri, 11-May-2012	—	Computer Lab
Mon, 14-May-2012	—	Tutorial
Tue, 15-May-2012	—	Lecture
Fri, 18-May-2012	—	Computer Lab
Mon, 21-May-2012	—	Tutorial
Tue, 22-May-2012	—	Lecture
Fri, 25-May-2012	—	Computer Lab
Mon, 28-May-2012	—	**No tutorial** (public holiday)
Tue, 29-May-2012	—	Lecture
Fri, 01-Jun-2012	—	Computer Lab
Mon, 04-Jun-2012	—	Tutorial
Tue, 05-Jun-2012	—	Lecture
Fri, 08-Jun-2012	—	Computer Lab
Mon, 11-Jun-2012	—	Tutorial
Tue, 12-Jun-2012	—	Lecture
Fri, 15-Jun-2012	—	Computer Lab
Mon, 18-Jun-2012	—	Tutorial
Tue, 19-Jun-2012	—	Lecture
Fri, 22-Jun-2012	—	Computer Lab
Mon, 25-Jun-2012	—	Tutorial
Tue, 26-Jun-2012	—	Lecture
Fri, 29-Jun-2012	—	Computer Lab
Mon, 02-Jul-2012	—	Tutorial
Tue, 03-Jul-2012	—	**No lecture**
Fri, 06-Jul-2012	—	Computer Lab
Mon, 09-Jul-2012	—	Tutorial
Tue, 10-Jul-2012	—	Lecture
Fri, 13-Jul-2012	—	Computer Lab

Quantum Reaction Dynamics

Lecture Contents

I. Concepts and methods

1. Brief review of quantum mechanics
2. Wavepacket dynamics
3. Numerical methods
4. Wigner representation

II. The nuclear Hamiltonian

1. Born-Oppenheimer separation
2. Coupled electronic states: Conical intersections
3. Adiabatic and diabatic representations

III. Interaction between molecules and light

1. The interaction Hamiltonian
2. Time-dependent perturbation theory

IV. Applications

1. Time-dependent simulation of absorption spectroscopy
2. Pump-dump spectroscopy
3. Wavepacket interferometry
4. Laser control ofmolecular dynamics
5. Strong field excitation
6. ...

Literature

- O. Kühn, J. Manz, I. Barth, H. Naundorf, Lecture Notes on Quantum Reaction Dynamics (Institut für Chemie, Freie Universität Berlin, 2006)
- D. J. Tannor, Introduction to Quantum Mechanics: A Time-Dependent Perspective, University Science Books (Sausalito, California, 2007)

Basic quantum mechanics

- C. Cohen-Tannoudji, B. Diu, F. Laloë, Quantum Mechanics, Wiley-Interscience (New York, 1977)
- E. Fick, Einführung in die Quantenmechanik, Aula-Verlag (Wiesbaden, 1988)
- A. S. Dawydow, Quantenmechanik, J. A. Barth (Leipzig, 1992)

Special topics

- W. P. Schleich, Quantum Optics in Phase Space, Wiley-VCH (Berlin, 2001)
- W. Domcke, D. R. Yarkony, H. Köppel (eds.), Conical Intersections: Electronic Structure, Dynamics & Spectroscopy, World Scientific (Singapore, 2004)
- W. Domcke, D. R. Yarkony, H. Köppel (eds.), Conical Intersections: Theory, Computation and Experiment, World Scientific (Singapore, 2011)
- M. Shapiro, P. Brumer, Principles of the Quantum Control of Molecular Processes, Wiley-Interscience (Hoboken, New Jersey, 2002)
- M. Shapiro, P. Brumer, Quantum Control of Molecular Processes, 2nd ed., Wiley-VCH (Weinheim, 2012)