

# Outline CHE512 Special Topics Course Fall 2004

## Instructor: J. Autschbach

### “Computation of Properties of Molecules and Crystals”

Three units, one credit hour each. The following combinations are possible:  
Only A, only B, only C, A + B, A + C, or A + B + C  
For each unit there will be one written exam (50% of the unit's grade) in week 5,  
and two assignments (25% of the unit's grade each).

#### Contents:

##### **Unit A** (5 weeks): *Static molecular properties*

The focus is on *NMR parameters* (chemical shifts & spin-spin coupling constants). Also: static polarizability, ESR parameters, calculation of IR vibrational frequencies. Theory and computational exercises (with the ADF quantum chemistry package)

Requirements: Basic knowledge of quantum theory, ideally – but not necessarily – CHE506

##### **Unit B** (5 weeks): *Time dependent linear properties*

The focus is on *the interaction of molecules with light*. Dynamic polarizability, optical rotation, electronic excitations, UV-VIS spectra, circular dichroism spectra, etc. Theory and computational exercises (with ADF)

Requirements: Unit A or an equivalent course (static perturbation theory). Please check with the instructor in case you intend to take unit B but not A.

##### **Unit C** (5 weeks): *Band structure theory, or “where are the bonds in solids?”*

The focus is on the *basics of band structure theory* and how to interpret its results in “chemical” terms. Simple Huckel (“tight binding”) theory and computational exercises (with the Stuttgart LMTO program).

Requirements: Same as Unit A. Unit C is independent of Units A and B.

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