

Welcome to Volker Staemmler's Group

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Our scientific interest is focussed on the quantum chemical treatment of electronically excited states of small molecules and on properties of clean and adsorbate-covered solid surfaces. Specific subjects are

- Spectroscopic properties of small molecules
- Magnetic exchange coupling in transition metal complexes
- X-ray emission and absorption spectra of molecules and solids
- Adsorption of small molecules on oxide surfaces

In these fields we are

- a) developing and improving quantum chemical ab initio methods which allow for accurate calculations
- b) performing numerical applications to specific systems and problems

Over the years, a wavefunction based quantum chemical ab initio program package has been developed in our group which is used for numerical calculations at different levels of accuracy: SCF, ROHF, CAS-SCF, CAS-CI, SOC-CI, MR-CI, MC-CEPA. In particular, our MC-CEPA program, which is an approximate multi-reference coupled cluster program, is able to yield results of almost experimental accuracy, even for systems with a complex electronic structure.

- curriculum vitae
- list of publications