The Location

Hotel Bredeney
Essen

Because of its central location the Hotel Bredeney is the ideal starting point to explore Essen, the Ruhr district and its environment. Life in Essen, the European Capital of Culture 2010, in the heart of the Ruhr district, is pulsating. Fascinating culture events, exciting sport events, exquisite restaurants and trendy business makes the modern Essen to one of the most beautiful and most alive cities of the region.

How to get there

Arrival by car:
Direction from Dusseldorf/Cologne/FRankfurt via A52:
Take the exit Essen-Haarzopf, then straight forward and at the second traffic lights turn right into the Theodor-Althoff-Strasse. The hotel is located on the left side.

Direction from Bremen/Hannover/Dortmund via A40:
Driving on the A40 change to the A52 direction Dusseldorf. After about 4 km take the exit Essen-Haarzopf/Margaretenhöhe. At the traffic lights turn left into the Theodor-Althoff-Strasse. The hotel is located on the left side.

Direction from Duisburg/Oberhausen via A40:
Driving on the A40 exit at Mülheim-Heißen. Turn right into the Frohnhauser Strasse. This street will become the Velauer Strasse and after that the Hatzperstrasse. At the Hatzperstrasse drive left into the Theodor-Althoff-Strasse. You will find the hotel on the right side.

Arriving with public transportation:
Arriving at Essen main station, take tram U11 (direction Messe/Gruga) and change at the terminus stop to bus 142 (direction Kettwig). Bus stop "Sommerburgstrasse" is in front of the hotel.

Computational Chemistry and Spectroscopy
Summer School 22.9. to 25.9. 2009
Chair of Theoretical Chemistry, Bonn, Germany

SFB 813 · SFB 624
GK 850 · IRTG 1422 · COST P15

\[ \frac{\partial^2 E}{\partial \lambda \partial \kappa} \bigg|_{\lambda = 0} = \sum_{\mu \nu} \frac{\partial P^{x \mu \nu}}{\partial \kappa} \langle \phi_{\mu} | \hat{h}, \phi_{\nu} \rangle + P^{x \mu \nu} \langle \phi_{\mu} | \hat{H}_{\kappa} | \phi_{\nu} \rangle \]
The course will start on the evening of Tuesday, Sept 22, 2009 with a keynote lecture “Magnetic Resonance Studies on Metalloenzymes: Hydrogenase and the Oxygen Evolving Complex” by Prof. Dr. Wolfgang Lubitz that will highlight the opportunities of present day quantum chemistry and its interaction with experimental investigations. The following three days will be devoted in equal parts to theoretical lectures and guided computational exercises. To this end, participants are required to bring their own laptops and pre-install the ORCA software that will be provided by the organizers. The material that will be covered in the lectures and practical courses will cover:

- Methods of quantum chemistry
- States, orbitals and Transitions
- Relativistic effects (mainly spin-orbit coupling)
- Ligand field theory as a guide to transition metal electronic structure
- Calculations on open-shell transition metals, oligonuclear clusters, biradicals and metal-radical systems.
- Calculation of EPR spectra
- Calculation of optical spectra

Handouts and reprints will be provided. The main part of the computational work will employ density functional theory, but wherever appropriate and feasible wavefunction based methods will also be used.

Participants are required to present a poster at the poster session that will take place on two evenings.