

Project 4.5 Ab initio investigations of Hund's Rule breaking organic molecules (theoretical)

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Institute: IF PAN

Unit: ON2.1

www: <http://www.ifpan.edu.pl/ON-2/on21.html>

Background:

The main scientific goal of the project bases on extensive ab initio computational explorations of novel, so-far unknown, organic compounds exhibiting the S1/T1 inversion in order to understand fundamental mechanisms and to determine electronic and nuclear factors that govern this unexpected and rare phenomenon. This is an almost completely unexplored field so far and the research will need the combination of chemical intuition in designing such systems with extensive computational work. Several wavefunction- and DFT- based methods of electronic structure theory such as MP2, ADC(2), CC2, CASSCF, UDFT, and TDDFT will be used for determination of molecular properties in the ground and in the lowest electronically excited states of theoretically designed polyatomic molecules.

Aim:

The technical aim of the project is related to future OLED application of these systems, and will involve computational optimization of the S1→S0 fluorescence intensity and wavelength of theoretically designed molecules with the restriction of a negative singlet-triplet energy gap. This part of the project will be performed in collaboration with Department of Theoretical Chemistry, Technical University of Munich.

The most promising molecular systems will be advised for synthesis and for spectroscopic investigation by collaborating experimental group in the Institute of Physics PAS as well as at Department of Chemistry, University of Washington, Seattle.

Requirements:

- basic knowledge of wavefunction- and DFT- based methods of electronic structure theory such as MP2, CC2, CASSCF, and TDDFT as well as sufficient proficiency in English is mandatory,
- some experience in running quantumchemical program packages like Gaussian, Turbomole or Molpro will be appreciated.

Funding:

Scholarship: grant funding of 5000 PLN per month, before subtracting obligatory employer and employee social security contributions (~15%), for 24 months. Afterwards, standard Polish PhD scholarship (about 3240 PLN/month net in years 3-4).

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