

Dr. Nicole Helbig

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Emmy Noether Young Investigators Group: Ab initio description of double and charge transfer excitations



„In the medium term the group will expand by participating in the Research Training Group RTG 1995 funded by the DFG. In the long term, I would like to broaden my research interests towards more applied topics.“

Research project:

The description of double and charge-transfer excitations within a density-functional framework is challenging since it requires a functional which is non-local in space and time. Especially the non-locality in time, i.e. a frequency dependence, is missing from currently available functionals.

Within this project we develop a frequency-dependent density functional. Moreover, as an alternative approach we employ reduced density-matrix functional theory, which has proven to be capable of solving many long-standing problems in density-functional theory.

The properties of all functionals are derived from exact calculations for one and two-dimensional model systems where the interacting Schrödinger equation can be solved without approximations for a small number of particles.

What is/has been the greatest challenge as head of a young investigators group:

Finding the right balance between research, teaching and administrative tasks

Start of funding period:

September 2011

End of funding period:

August 2016

Budget:

ca. 200000 Euros/year

Staff:

1 Postdoc, 1 Phd student

Cooperations:

University of the Basque Country San Sebastian, National Hellenic Research Foundation, Durham University

Further information:

[Young Investigator Group Dr. Helbig](#)