

News

Ph.D. position within NCN Preludium BIS-2 project (deadline July 30,2021) [Offer description](#)

Four-year Ph.D. position starting October 1. 2021, available in the Institute of Physics Nicolaus Copernicus University in Toruń, Poland under PRELUDIUM BIS-2 Project No. 2020/39/O/ST4/00005 entitled "From Coupled Cluster theory to accurate semi-local Kohn-Sham correlation functional" (leader prof. dr. hab. Ireneusz Grabowski ig@fizyka.umk.pl). [MORE DETAILS \(PDF\)](#)

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- S. Śmiga, Sylwia Siecińska, I. Grabowski
"From simple molecules to nanotubes. Reliable predictions of ionization potentials from the MP2-SCS methods."
New J. Phys. 22 (2020), 083084-1
- S. Śmiga, I. Grabowski, Mateusz Witkowski, Bastien Mussard, Julien Toulouse
"Self-consistent range-separated density-functional theory with second-order perturbative correction via the optimized-effective-potential method"
J. Chem. Theory Comput. 16 (2020), 211-223
- S. Śmiga, Volodymyr Marusiak, I. Grabowski, Eduardo Fabiano
"The ab initio density functional theory applied for spin-polarized calculations"
J. Chem. Phys. 152 (2020), 054109
- Eduardo Fabiano, S. Śmiga, Sara Giarrusso, Tim Daas, Fabio Della Sala, I. Grabowski, Paola Gori-Giorgi
"Investigation of the exchange-correlation potential of functionals based on the adiabatic connection interpolation"
J. Chem. Theory Comput. 15 (2019), 1006-1015
- S. Śmiga, I. Grabowski
"The spin-component-scaled Δ MP2 parametrization: towards a simple and reliable method for ionization energies"
J. Chem. Theory Comput. 14 (2018), 4780-4790

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