Quantum Chemical Treatment of Strongly Correlated Magnetic Systems Based on Heavy Elements

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Overall research goals:

The objective of this project over the years has been to develop novel quantum chemical methods and employ them to study the chemistry of systems containing actinides, and transactinides. We have focused on their electronic and spectroscopic properties, their reactivity and utilization as single molecule magnets.
We have developed wave-function based methods that are optimal to treat strongly correlated systems, namely systems with many electronic configurations that are all important and should be treated on an equal foot. Moreover, relativistic effects have to be included in the model, with special focus on spin-orbit coupling. We have derived our theories and developed our codes and made them available to the community as parts of open source packages. We have modelled systems in collaboration with experimentalists in the program, so that we could address some of the questions that are relevant to this community. We have also worked in collaboration with people at Lawrence Livermore National Laboratories on a project on super-heavy atoms. We hope that our theoretical predictions will inspire novel experiments. We have trained about 10 students/postdocs during this period, which are now faculty, researchers at national laboratories and in companies.

Publications supported by this project

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