Gabriele Fabbro

Personal Informations

Full name: Gabriele Fabbro
Date and place of birth: 10 November 1998, Pordenone (Italy)
Citizenship: Italian
Current job position: PhD student at Universitè Paul Sabatier (Toulouse, France)
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Education

Universite' Paul Sabatier III — **Nov. 2022 – Ongoing**
PhD in Theoretical Chemistry (Adv: Dr. Trond Saue) — *Toulouse, France*

Universita' degli Studi di Trieste — **Oct. 2020 – Oct. 2022**
European Master in Theoretical Chemistry and Computational Modelling [110/110 cum laude] — *Trieste, Italy*

Universita' degli Studi di Trieste — **Oct. 2017 – Sep. 2020**
Bachelor degree in Chemistry [110/110] — *Trieste, Italy*

Istituto Tecnico Settore Tecnologico J.F.Kennedy — **Sep. 2014 – Aug. 2017**
Pordenone, Italy

Languages

Italian: Mother tongue
English: B2

Technical Skills

Languages: Fortran 90/95
Text Editors: Word, LaTeX
Operating systems: Linux, MacOS

Relevant Professional Experience

Master thesis research: During my master thesis period, held in Toulouse at the Paul Sabatier University from March to July 2022 under the supervision of Dr. Trond Saue, I dealt with the issue of calculating and analyzing the electric field gradient at nuclear positions in a relativistic scheme. Nuclei having a nuclear quantum spin number $I > 1/2$ possess a nuclear electric quadrupole moment, which couples with the electric field gradient generated by the other electrons and nuclei present. This coupling is quantifiable by the nuclear quadrupole coupling constant (NQCC) which can be determined experimentally. Combining the experimental approach and the theoretical approach through accurate calculations of the electric field gradient it is possible to obtain the electric quadrupole moment of a nucleus, which turns out to be an important piece of physical information. The electric field gradient also makes it possible to provide important chemical information, such as the nature of a bond involving two atoms.

PhD thesis research: The thesis is part of the project HAMP-vQED [Highly Accurate Molecular Properties using variational Quantum Electrodynamics] funded by an ERC Advanced Grant. The building blocks of chemistry are organized in the periodic table, which requires quantum mechanics for its understanding. In the 1980s it was realized that in order to correctly describe the heavy elements in the lower part of the periodic table, the special theory of relativity had to be invoked. Does chemistry need more physics? The HAMP-vQED project will investigate the possible role of quantum electrodynamics (QED) in chemistry. It will provide a protocol for highly accurate calculations of molecular properties, with particular attention to properties that probe the electron density in the close vicinity of atomic nuclei, where the QED-effects are created. The HAMP-vQED project adheres to the general framework of quantum chemistry by seeking a variational (non-perturbative) approach using local (Gaussian) basis functions (more information can be found here: https://dirac.ups-tlse.fr/hamp-vqed/doku.php). Coupled cluster (CC) theory plays a central part in the HAMP-vQED project since it provides electron correlation in an efficient and systematic manner, which is indispensable for the accurate calculation of molecular properties. As platform for further development we will use the DIRAC code for relativistic molecular calculations . The DIRAC code features two coupled cluster modules: the RELCCSD module and the more recent EXACORR module ; the latter is geared for massively parallel calculations, whereas the former benefits from an extensive treatment of molecular symmetry. It is planned to merge the two codes during the HAMP-vQED project, taking the best of both worlds, and to provide powerful tools for further CC development. The RELCCSD module allows the calculation of expectation values as well as excitation, ionization and electron attachment energies , and much of this functionality is currently being added to the EXACORR module. The thesis focuses on the calculation of linear response functions, which are second-derivatives of the energy. Such properties include polarizabilities, magnetizabilities and NMR parameters. As

already mentioned, we shall in particular be interested in molecular properties that probe the electron density in the vicinity of nuclei. This is where QED-effects are generated. The calculation of magnetic properties is in particular challenging, since they in relativistic response theory involve the solutions (orbitals) of the Dirac equation of negative-energy. Such solutions are normally excluded from conventional relativistic molecular calculations, but have now to be somehow taken into account.

Seminars and Schools

Molecular Response Properties Summer School | *Stockholm, Sweden* **June 2023**

Conducting your doctoral project | *Toulouse, France* **Mar. 2023**

Introduction aux systèmes de Calcul HPC et prise en main du système Olympe | *Toulouse, France* **Jan. 2023**

European Summerschool in Quantum Chemistry (ESQC22) | *Torre Normanna, Italy* **Sep. 2022**

Winter School for advanced sciences of Luchon: Tutorials in Theoretical Chemistry | *Aspet, France* **Feb. 2022**

Advanced Computational Techniques | *Paris, France* **Nov. 2022**

Advanced methods in Electronic Structure, Dynamics and Molecular Modelling | *Toulouse, France* **Sep. 2021**

Scientific oral communications

26th DIRAC Working Group Meeting | *Odense, Denmark* **May-June 2023**

- Scientific talk: Analysis and calculation of electric field gradient in relativistic framework.

Molecular Response Properties Summer School | *Stockholm, Sweden* **June 2023**

- Poster session: Beyond the Dailey-Townes model: chemical information from the electric field gradient.

European Summerschool in Quantum Chemistry (ESQC22) | *Torre Normanna, Italy* **Sep. 2022**

- Poster session: Analysis and calculation of electric field gradient in relativistic framework.