

ERC PTEROSOR

Data Management Plan

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(Dated: June 30, 2020)

I. PROJECT DETAILS

Title	PTEROSOR
Funder	European Research Council, ERC
Number	863481
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II. SUMMARY

Catalysis and solar cell technologies are underpinned by a fundamental process: that of exciting systems to a higher energy level than the ground state. Defining an effective method to achieve this that also provides accurate energies of the excited states is often a challenge. The EU-funded PTEROSOR project will tackle this fundamental problem using mathematical techniques. The researchers' novel approach for measuring the energies of excited states and defining wave functions in molecular systems will hinge on the use of a general class of Hamiltonians with parity-time (PT) symmetry. The gateway between ground and excited states will be provided by exceptional points which lie at the boundary between broken and unbroken PT-symmetric regions.

III. RESEARCH OUTPUTS

1. QuAcK (Software)

2. Quantum Package (Software)
3. Notebooks (Interactive Resource)
4. Textual data (Text)

IV. DATASET SUMMARY

QuAcK is a small quantum chemistry package written in Fortran by the coordinator of the project. It is mostly used for prototyping. The size of the archive containing the source code is around 4MiB, and is composed of Fortran source files, Python and Bash scripts, and Makefiles.

Quantum Package is an open-source quantum chemistry package for performing selected configuration interaction calculations with perturbation theory for molecules and solids. The project was initiated in 2015 at the LCPQ, and it is now developed on three sites : Toulouse (LCPQ Toulouse, France), Paris (LCT Paris, France) and Argonne (USA). Quantum Package is one of the flagship codes of the TREX European Center of Excellence. The size of the archive is around 11MiB, and is composed of IRPF90 source files, Python, Bash scripts, Makefiles and standard atomic basis sets and pseudo-potentials.

All along the project, Mathematica / Jupyter / Org-mode notebooks will be produced by researchers and students. Each notebook will take a few megabytes.

PDF files for reports, publications, presentations and posters will be produced in this project. Each pdf file will take a few megabytes. Care will be taken to maintain the size of these documents as small as possible.

V. FAIR DATA AND RESOURCES

A. Making data findable

QuAcK is hosted on GitHub (<https://github.com/pfloos/quack>), with a mirror on the Git repository of the LCPQ (<https://git.irsamc.ups-tlse.fr/scemama/quack>). The latest version was uploaded on Zenodo ([doi:10.5281/zenodo.3745928](https://doi.org/10.5281/zenodo.3745928)).

Quantum Package is hosted on GitHub (<https://github.com/QuantumPackage/qp2>), with a mirror on the Git repository of the LCPQ (<https://git.irsamc.ups-tlse.fr/>

LCPQ/qp2). The latest version of the program was presented in a [peer-reviewed article](#), and the corresponding preprint was published on [ArXiv](#) and [HAL](#). The associated source code was uploaded on Zenodo ([doi:10.5281/zenodo.3677565](https://doi.org/10.5281/zenodo.3677565)), and the source code contains a `CITATION.cff` file providing metadata in standard YAML format. Quantum Package has its dedicated website (<https://quantumpackage.github.io/qp2>) providing links to the GitHub repository, the documentation (<https://quantum-package.readthedocs.io>), and video tutorials hosted on a YouTube channel (<https://www.youtube.com/channel/UC3a7Yakg9gk36G3HKDIFaYw>). Quantum Package has also a twitter account (@quantum_package).

All the notebooks will be versioned in the Git repository of the LCPQ (<https://git.irsamc.ups-tlse.fr>), publicly accessible. These documents will be archived on Figshare or Zenodo, and the DOIs will be provided in publications.

The \LaTeX source files relative to reports, publications, presentations and posters will be versioned in the Git repository of the LCPQ, publicly accessible.

We plan to submit all the source codes involved in this project to the [Software Heritage](#) archive.

A web site for the project will be created, centralizing all the links to the archived data. Care will be taken to provide useful metadata in the HTML headers to help the search engines reference this web site.

B. Making data openly accessible

QuAcK is released under the GPL v3 license. Quantum Package is released under the AGPL v3 license.

Both GitHub repositories are set up to automatically upload on Zenodo every new release. For each publication requiring a modification of the source code, a release will be made and the Zenodo DOI will be cited.

The project doesn't require any part of the codes to be confidential.

C. Making data interoperable

Standard xyz format is used for atomic coordinates and GAMESS/US format for atomic basis sets is used. The Basis Set Exchange (BSE) website (<https://www.basissetexchange>.

org) provides data in this format.

Quantum Package is already interfaced with multiple codes of the community (GAMESS, Molpro, Gaussian, QMCPack, QMC=Chem, ...)

QuAcK operates internally with text files, using the same conventions as Quantum Package. Hence, the two codes are compatible and easily interoperable.

D. Increase data reuse

Along the project, the code will be structured in independent inter-operating components to make easier the extraction of a particular feature of the package.

Continuous integration will be set up to guarantee that the package is functional in the main branch. Developments will be made in a secondary development branch.

E. Allocation of resources and data security

The mirroring of the GitHub repository in the institute of the coordinator provides a backup of both QuAcK and Quantum Package.

The automatic upload of new releases on Zenodo provides secure storage and long-term preservation of the source code.

We also plan to upload the code in the Software Heritage digital archive.