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Quantum Package 2.0 : a web demo

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QUANTUM PACKAGE is an open-source programming environment for quantum chemistry developed at the Laboratoire de Chimie et Physique Quantiques (LCPQ) by Anthony Scemama and coworkers.[1] It is specially designed for wave function methods, and its main goal is the development of determinant-driven selected configuration interaction (sCI) methods and multireference second-order perturbation theory (PT2). The second version is also designed to be user- and developer-friendly, easy to install, and to extend with plugins thanks to the Implicit Reference to Parameters (IRP) paradigm. Following this philosophy, we have developed a demo available directly on the web with any modern web browser. Thanks to this functionality, one can simply use a web browser to test Quantum Package 2.0 and all the quantum chemistry methods available right out of the box. In this poster, I will explain and illustrate what are the most interesting features of Quantum Package 2.0 and describe the demo architecture. A live presentation of Quantum Package will be available on demand.

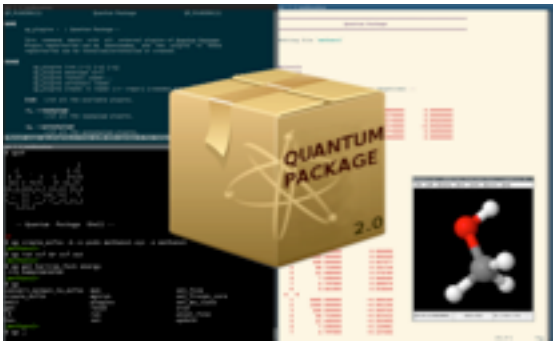

Figure 1. Quantum Package 2.0

Mots-clés : Quantum chemistry, Selected Configuration Interaction, Quantum Package, Implicit Reference to Parameters, Docker.

Références

[1] Y. Garniron et al, ***Journal of Chemical Theory and Computation***, *15* (6), 3591-3609 (2019).