

HQS Introduces an Update to the Open-Source Tool Active Space Finder, Collaborating with Covestro

HQS Quantum Simulations (HQS), a leading provider of quantum simulation solutions, announces the release of an update to its open-source tool, the Active Space Finder (ASF). Developed in collaboration with Covestro, a global player in the field of polymer materials, this update aims to enhance chemical simulations by simplifying the selection of active spaces in molecules.

Karlsruhe, 08.07.2024: The Active Space Finder (ASF) is a powerful set of functions designed for the (semi-)automatic selection of active spaces in molecules, particularly for methods such as CASSCF (Complete Active Space Self-Consistent Field). Selecting the appropriate set of active orbitals can be a complex task that requires significant expertise. Recognizing this challenge, HQS and Covestro have been working together since 2020 to develop a tool that makes such calculations easier and more accessible to both expert and non-expert users. The initial version of the ASF has been available on GitHub since 2021, and users can now download the improved version.

The updated version of the Active Space Finder offers improved robustness and user-friendliness of results. It provides multiple suggestions for active orbitals, allowing users to choose the most suitable option for their specific needs.

“By analyzing the interaction and entanglement of electrons in the orbitals, the Active Space Finder enables a deeper understanding of molecular systems. We will leverage this tool to gain valuable insights and improve our understanding of complex chemical processes in the field of polymer materials”, says Dr. Christian Gogolin, Head of High Performance & Quantum Computing at Covestro.

"We are excited to collaborate with Covestro on the development of the Active Space Finder," said Dr. Peter Pinski, Stack Leader Quantum Chemistry at HQS Quantum Simulations and Project Manager. "This update represents a significant step forward in simplifying multi-reference calculations and making them more accessible to researchers in the field of quantum chemistry."

The Active Space Finder also has a strong connection to the emerging field of quantum computing. In the era of Noisy-Intermediate-Scale-Quantum (NISQ) devices, employing early-stage quantum technologies for quantum chemistry applications requires reducing problems to their most important degrees of freedom. The ASF aims to identify the crucial parts of a molecular system that need to be treated at the most advanced quantum mechanical level.

The Active Space Finder has been an integral part of several publicly funded projects, including MANIQU, PlanQK, and PhoQuant, further demonstrating its value and versatility in the scientific community.

For more information about the Active Space Finder and to download the Open Source Tool, please visit:
www.github.com/HQSquantumsimulations/ActiveSpaceFinder

More information:

www.covestro.com.

<https://quantumsimulations.de/news/hqs-provides-a-setup-for-the-simulation-of-chemical-processes-in-the-quantum-computing-project-qc-4-bw>

<https://quantumsimulations.de/case-studies/maniqu>

About HQS Quantum Simulations

HQS Quantum Simulations represents a new era in quantum simulation. We harness the potential of quantum mechanics to develop innovative industrial applications. Our solutions are based on innovative approaches to accurate and efficient material prediction and analysis at the quantum level. HQS software is used in the pharmaceutical and chemical industries, as well as in the development and research of quantum computers, sensors, optical components, and laser applications.

About Covestro

Covestro is one of the world's leading manufacturers of high-quality polymer materials and their components. With its innovative products, processes and methods, the company helps enhance sustainability and the quality of life in many areas. Covestro supplies customers around the world in key industries such as mobility, building and living, as well as the electrical and electronics sector. In addition, polymers from Covestro are also used in sectors such as sports and leisure, telecommunications and health, as well as in the chemical industry itself.

The company is geared completely to the circular economy. In addition, Covestro aims to achieve climate neutrality for its Scope 1 and Scope 2 emissions by 2035, and the Group's Scope 3 emissions are also set to be climate neutral by 2050. Covestro generated sales of EUR 14.4 billion in fiscal year 2023. At the end of 2023, the company had 48 production sites worldwide and employed approximately 17,500 people (calculated as full-time equivalents).

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