Contribution ID: **105** Type: **Poster**

Simulating Vibronic Spectra by Direct Application of Doktorov Formulae on Superconducting Quantum Simulator

Tuesday, 7 May 2024 17:30 (1h 30m)

In this work, a direct quantum implementation of the Doktorov formulae for calculating the vibronic spectrum of molecules under the harmonic approximation is presented. The classically hard problem of estimating the Franck-Condon (FC) factors is solved by using the Duschinsky matrices as the only input via the Doktorov quantum circuit. This approach offers the advantage of avoiding basis changes and symmetry dependencies, while making use of the inherent computational advantages of quantum computers. In other words, it is a general method that can be extended to molecules of any size. Its application is demonstrated with the three-atom molecules SO2 and ZnOH.

References

E. Doktorov et al. Dynamical symmetry of vibronic transitions in polyatomic molecules and the Franck-Condon principle. J. Mol. Spectrosc. 1977, 64, 302–326.

Abstract category

Primary author: Mr OLARTE HERNANDEZ, Renato (University of Namur)

Co-authors: SOLDERA, Armand (University of Sherbrooke); CHAMPAGNE, Benoît (University of Namur)

Presenter: Mr OLARTE HERNANDEZ, Renato (University of Namur)

Session Classification: Poster session