Contribution ID : **59** Type : **Poster Presentation**

EuCompChem2025 – Federico Rossi – Oral

The description of conical intersections is a key requirement in non-adiabatic molecular dynamics. Standard Hartree-Fock and Density Functional Theory, with the corresponding TDHF and TDDFT methods for excited states, are unable to describe ground state conical intersections, as the ground state is decoupled from the excited states. As system size increases, multiconfigurational methods become unfeasible and the need for a cost-efficient method becomes crucial.

Here we present a modified Hartree-Fock method, where the ground state is optimized in a lower-dimensional subspace, removing the projection along selected Hessian eigenvectors. In a final step, the energies of the ground and excited states are obtained by diagonalizing the Hamiltonian. Several applications will be presented and compared with TDHF and TDDFT in the Tamm-Dancoff approximation. A similar computational framework has recently been used to develop a coupled cluster method that correctly accounts for the geometric phase effect and avoids bifurcations of the solutions to the ground state equations.

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