Enzo Monino

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Education

PhD in Theoretical Chemistry Université de Toulouse (France) Master's degree in Theoretical Chemistry Université de Montpellier (France) Bachelor's degree in Physics and Chemistry Université de Montpellier (France) 2018 - 2020 2015 - 2018

Experience

Institut Charles Gerhardt Montpellier (ICGM)

Feb 2020 - Jul 2020

2nd year of Master degree internship

Montpellier, France

- Studied Time-Dependent Density Functional Theory (TD-DFT).
- Studied orbital relaxation in the context of molecular electronic transitions computation.

Laboratoire Univers et Particules de Montpellier (LUPM)

May 2019 - Jul 2019

1st year of Master degree internship

Montpellier, France

- Studied quantum dynamics by wave packets.
- Computation of bound states of ${\rm HeH_2}^+$ complex using the Multi Configuration Time Dependent Hartree (MCTDH) approach.

Posters

Symmetry breaking in Green's function methods: the case of H_2

2nd General Meeting of the GDR NBODY, Toulouse (France), Jan 10-13, 2022

E. Monino and P. F. Loos.

Reference Energies for Cyclobutadiene: Automerization and Excited States

Meetings of Francophone Theoretical Chemists, Bordeaux (France), Jun 27 - Jul 01, 2022

E. Monino, M. Boggio-Pasqua, A. Scemama, D. Jacquemin and P. F. Loos.

Unphysical Discontinuities, Intruder States and Regularization in GW Methods

World Association of Theoretical and Computational Chemists (WATOC), Vancouver (Canada), Jul 03 - 08, 2022

E. Monino and P. F. Loos.

Spin-Conserved and Spin-Flip Optical Excitations From the Bethe-Salpeter Equation Formalism

New Horizons In Scientific Software (NHISS), Jeju (South Korea), Dec 12-15,2022

E. Monino and P. F. Loos.

Presentation

Reference Energies for Cyclobutadiene: Automerization and Excited States

"Theory, Modeling and Simulations" Days, Rennes (France), Oct 13 - 14, 2022

E. Monino, M. Boggio-Pasqua, A. Scemama, D. Jacquemin and P. F. Loos.

Publications

QCMATH: Mathematica modules for electronic structure calculations,

arXiv, 2308.14890 [physics.chem-p] (2023).

E. Monino, A. Marie and P. F. Loos.

Connections and performances of Green's function methods for charged and neutral excitations,

- J. Chem. Phys. 159, 034105 (2023).
- **E.** Monino and P. F. Loos.

Connections between many-body perturbation and coupled-cluster theories,

- J. Chem. Phys. 157, 231102 (2022).
- R. Quintero-Monsebaiz, E. Monino, A. Marie, and P. F. Loos.

Reference Energies for Cyclobutadiene: Automerization and Excited States

- J. Phys. Chem. A 126, 4664 (2022).
- E. Monino, M. Boggio-Pasqua, A. Scemama, D. Jacquemin, and P. F. Loos.

Unphysical discontinuities, intruder states and regularization in GW methods

- J. Chem. Phys. 156, 231101 (2022).
- **E.** Monino and P. F. Loos.

Spin-Conserved and Spin-Flip Optical Excitations from the Bethe-Salpeter Equation Formalism

- J. Chem. Theory Comput. 17, 2852 (2021).
- E. Monino and P. F. Loos.

Upper bound for the charge transferred during a molecular electronic transition — Insights from matrix analysis

(preprint) (2021).

E. Monino and T. Etienne.

Technical skills

Programming Languages/Tools Fortran, Mathematica, Languages Fortran, Languages Fortran,