

Enzo Monino

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<https://enzomonino.github.io/>

Education

PhD in Theoretical Chemistry <i>Université de Toulouse (France)</i>	<i>2020 - 2023</i>
Master's degree in Theoretical Chemistry <i>Université de Montpellier (France)</i>	<i>2018 - 2020</i>
Bachelor's degree in Physics and Chemistry <i>Université de Montpellier (France)</i>	<i>2015 - 2018</i>

Experience

Postdoctoral position <i>J. Heyrovsky Institute of Physical Chemistry</i>	<i>Jan 2024 - Today</i> <i>Prague, Czech Republic</i>
<ul style="list-style-type: none">• Quantum chemistry on quantum computers.• Density Matrix Renormalization Group (DMRG).	
Institut Charles Gerhardt Montpellier (ICGM) <i>2nd year of Master degree internship</i>	<i>Feb 2020 - Jul 2020</i> <i>Montpellier, France</i>
<ul style="list-style-type: none">• Study of Time-Dependent Density Functional Theory (TD-DFT).• Study of orbital relaxation in the context of molecular electronic transitions computation.	
Laboratoire Univers et Particules de Montpellier (LUPM) <i>1st year of Master degree internship</i>	<i>May 2019 - Jul 2019</i> <i>Montpellier, France</i>
<ul style="list-style-type: none">• Study of quantum dynamics by wave packets.• Computation of bound states of 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.

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, L^AT_EX, Bash

Languages

French (native), English (TOIEC C1 certification)

Quantum chemistry softwares

Gaussian, QChem