Fábris Kossoski

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Webpages: ResearcherID | Google scholar | ORCID | Research Gate

Research interests

- Electron-molecule collisions
- Electronic structure theory
- Photophysics and photochemistry
- Mixed quantum-classical methods
- Software development for theoretical chemistry

Professional experience

11/2020 – present **Postdoctoral researcher**
Laboratoire de Chimie et Physique Quantiques
Université Paul Sabatier, Toulouse, France
Workgroup of Pierre-François Loos

11/2018 – 09/2020 **Postdoctoral researcher**
Institut de Chimie Radicalaire
Aix Marseille Université, Marseille, France
Workgroup of Mario Barbatti

05/2017 – 04/2018 **Postdoctoral researcher internship**
Institut de Chimie Radicalaire
Aix-Marseille Université, Marseille, France
Workgroup of Mario Barbatti

05/2016 – 04/2017
05/2018 – 10/2018 **Postdoctoral researcher**
"Gleb Wataghin" Physics Institute
State University of Campinas, Campinas, Brazil
Workgroup of Marco A. P. Lima

Education

03/2012 – 02/2016 **PhD in Physics**
Thesis: *Dynamics of temporary ions of halogenated biomolecules*
Physics Institute
University of São Paulo, São Paulo, Brazil
Supervisor: Márcio T. do N. Varella

03/2010 – 02/2012 **Master in Physics**
Thesis: *Elastic electron scattering by isomers of $C_2H_2Cl_2$, $C_4H_4N_2$, and C_3H_3NX (X=NH, O, S)*
Physics Department
Federal University of Paraná, Curitiba, Brazil
Supervisor: Márcio H. F. Bettega

03/2006 – 02/2010 **Degree in Physics**
Physics Department
Federal University of Paraná, Curitiba, Brazil

Research metrics

Number of peer-reviewed publications	36
Peer-reviewed publications as first and/or corresponding author	21
Peer-reviewed publications as corresponding author	16
Peer-reviewed publications as first author	13
Number of citations (Web of Science)	355
Number of citations (Google Scholar)	488
H-index (Web of Science)	12
H-index (Google Scholar)	13
Talks in conferences	13
Invited talks in conferences	7

Publications

Corresponding authors are indicated by *****

- **Preprints**

1. A. G. Falkowski, R. F. da Costa, M. A. P. Lima, A. d. A. Cadena, R. Pocoroba, R. Jones, M. Mathur, J. G. Childers, M. A. Khakoo*, **F. Kossoski***. *A theoretical and experimental investigation of electronic excitation of benzene by electron impact.*

- **Publications in peer-reviewed scientific journals**

36. F. Kossoski*, P.-F. Loos*. *State-Specific Configuration Interaction for Excited States.* J. Chem. Theory Comput. 19, 2258 (2023).

35. Y. Damour*, R. Quintero-Monsebaiz, M. Caffarel, D. Jacquemin, **F. Kossoski**, A. Scemama, P.-F. Loos*. *Ground- and Excited-State Dipole Moments and Oscillator Strengths of Full Configuration Interaction Quality.* J. Chem. Theory Comput. 19, 221 (2023).

34. A. d. A. Cadena, A. G. Falkowski, R. Pocoroba, R. Jones, M. Mathur, J. G. Childers, A. S. Barbosa, M. H. F. Bettega, R. F. da Costa, M. A. P. Lima, **F. Kossoski***, M. A. Khakoo*. *Cross sections for elastic electron scattering by benzene at low and intermediate energies.* Phys. Rev. A 106, 062825 (2022).

33. M. Barbatti*, M. Bondanza, R. Crespo-Otero, B. Demoulin, P. O. Dral, G. Granucci, **F. Kossoski**, H. Lischka, B. Mennucci, S. Mukherjee, M. Pederzoli, M. Persico, M. Pinheiro Jr, J. Pittner, F. Plasser, E. S. Gil, L. Stojanovic. *The Newton-X platform: new software developments for surface hopping and nuclear ensembles.* J. Chem. Theory Comput. 18, 6851 (2022).

32. A. I. Lozano*, **F. Kossoski***, F. Blanco, P. Limão-Vieira, M. T. do N. Varella, G. García. *Observation of Transient Anions That Do Not Decay through Dissociative Electron Attachment: New Pathways for Radiosensitization.* J. Phys. Chem. Lett. 13, 30, 7001 (2022).

31. F. Kossoski*, Y. Damour, P.-F. Loos*. *Hierarchy Configuration Interaction: Combining Seniority Number and Excitation Degree.* J. Phys. Chem. Lett. 13, 19, 4342 (2022).

30. A. G. Falkowski, R. F. da Costa, **F. Kossoski***, M. J. Brunger, M. A. P. Lima. *Electronic excitation of benzene by low energy electron impact and the role of higher lying Rydberg states.* Eur. Phys. J. D 75, 310 (2021).

29. Y. Damour, M. Véril, **F. Kossoski**, M. Caffarel, D. Jacquemin*, A. Scemama*, P.-F. Loos*. *Accurate full configuration interaction correlation energy estimates for five- and six-membered rings.* J. Chem. Phys. 155, 134104 (2021).

28. A. Marie, **F. Kossoski**, P.-F. Loos*. *Variational coupled cluster for ground and excited states.* J. Chem. Phys. 155, 104105 (2021).

27. J. C. Ruivo, **F. Kossoski**, M. T. do N. Varella*. *Anion states of halocamphor molecules: insights into chirally sensitive dissociative electron attachment.* Phys. Chem. Chem. Phys. 23, 17616 (2021).

26. F. Kossoski*, A. Marie, A. Scemama, M. Caffarel, P.-F. Loos*. *Excited States from State-Specific Orbital-Optimized Pair Coupled Cluster.* J. Chem. Theory Comput. 17, 4756 (2021).

25. M. Mendes*, **F. Kossoski***, A. I. Lozano, J. Pereira-da-Silva, R. Rodrigues, J. Ameixa, N. C. Jones, S. V. Hoffmann, F. Ferreira da Silva. *Excited states of bromopyrimidines probed by VUV photoabsorption spectroscopy and theoretical calculations.* Int. J. Mol. Sci. 22(12), 6460 (2021).

24. J. Pereira-da-Silva, M. Mendes*, **F. Kossoski***, A. I. Lozano, R. Rodrigues, N. C. Jones, S. V. Hoffmann, F. Ferreira da Silva. *Perfluoro effect on the electronic excited states of para-benzoquinone revealed by experiment and theory.* Phys. Chem. Chem. Phys. 23, 2141 (2021).

23. M. Kiataki, M. T. do N. Varella, M. H. F. Bettega, **F. Kossoski***. *Shape Resonances and Elastic Cross Sections in Electron Scattering by CF_3Br and CF_3I.* J. Phys. Chem. A 124, 42, 8660 (2020).

22. A. I. Lozano, L. S. Maioli, B. Pamplona, J. Romero, M. Mendes, F. Ferreira da Silva, **F. Kossoski**, M. Probst, D. Süß, M. H. F. Bettega, G. García, P. Limão-Vieira*. *Selective bond breaking of halothane induced by electron transfer in potassium collisions.* Phys. Chem. Chem. Phys. 22, 23837 (2020).

21. F. Kossoski*, M. Barbatti*. *Nonadiabatic dynamics in multidimensional complex potential energy surfaces.* Chem. Sci. 11, 9827 (2020).

20. A. G. Falkowski, M. A. P. Lima, **F. Kossoski***. *Electronic excitation of ethanol by low-energy electron impact.* J. Chem. Phys. 152, 244302 (2020).

19. L. S. Maioli, **F. Kossoski***, M. H. F. Bettega. *Low-energy electron scattering by cyanamide: anion spectra and dissociation pathways.* Phys. Chem. Chem. Phys. 22, 7894 (2020).

18. H. Lischka*, R.Shepard*, T. Müller, P. G. Szalay, R. M. Pitzer, A. J. A. Aquino, M. M. Araújo do Nascimento, M. Barbatti, L. T. Belcher, J.-P. Blaudeau, I. Borges Jr., S. R. Brozell, E. A. Carter, A. Das, G. Gidofalvi, L. González, W. L. Hase, G. Kedziora, M. Kertesz, **F. Kossoski**, F. B. C. Machado, S. Matsika, S. A. do Monte, D. Nachtigallova, R. Nieman, M. Oppel, C. A. Parish, F. Plasser, R. F. K. Spada, E. A. Stahlberg, E. Ventura, D. R. Yarkony, Z. Zhang. *The Generality of the GUGA MRCI Approach in COLUMBUS for Treating Complex Quantum Chemistry.* J. Chem. Phys. 152, 134110 (2020).

17. G. M. Moreira, **F. Kossoski**, M. H. F. Bettega, R. F. da Costa*. *Electronic excitation of the $^3B_2$ state of thiophene molecule by low-energy electron collisions.* J. Phys. B: At. Mol. Opt. Phys. 53, 085002 (2020).

16. F. Kossoski*, M. T. do N. Varella*, M. Barbatti*. *On-the-fly dynamics simulations of transient anions.* J. Chem. Phys. 151, 224104 (2019).

15. R. F. da Costa*, J. C. Ruivo, **F. Kossoski**, M. T. do N. Varella, M. H. F. Bettega, D. B. Jones, M. J. Brunger, M. A. P. Lima. *An ab initio investigation for elastic and electronically inelastic electron scattering from para-benzoquinone.* J. Chem. Phys. 149, 174308 (2018).

14. F. Kossoski*, M. Barbatti*. *Nuclear Ensemble Approach with Importance Sampling.* J. Chem. Theory Comput. 14, 3173 (2018).

13. D. B. Jones, R. F. da Costa, **F. Kossoski**, M. T. do N. Varella, M. H. F. Bettega, G. García, F. Blanco, R. D. White, M. A. P. Lima*, M. J. Brunger*. *Integral elastic, vibrational-excitation, electronic-state excitation, ionization, and total cross sections for electron scattering from para-benzoquinone.* J. Chem. Phys. 148, 204305 (2018).

12. D. B. Jones*, R. F. da Costa, **F. Kossoski**, M. T. do N. Varella, M. H. F. Bettega, F. Ferreira da Silva, P. Limão-Vieira, G. García, M. A. P. Lima*, R. D. White, M. J. Brunger. *Electron-impact electronic-state excitation of para-benzoquinone.* J. Chem. Phys. 148, 124312 (2018).

11. D. B. Jones, F. Blanco, G. García, R. F. da Costa, **F. Kossoski**, M. T. do N. Varella, M. H. F. Bettega, M. A. P. Lima, R. D. White, M. J. Brunger*. *Elastic scattering and vibrational excitation for electron impact on para-benzoquinone.* J. Chem. Phys. 147, 244304 (2017).

10. L. M. Cornetta, **F. Kossoski**, M. T. do N. Varella*. *Transient anion spectra of the potential radiosensitizers 5-cyanateuracil and 5-thiocyanateuracil.* J. Chem. Phys. 147, 214310 (2017).

9. F. Kossoski*, M. T. do N. Varella*. *How does methylation suppress the electron induced decomposition of 1-methyl-nitroimidazoles?* J. Chem. Phys. 147, 164310 (2017).

8. F. Kossoski*, M. T. do N. Varella*. *Precursor anion states in dissociative electron attachment to chlorophenol isomers.* J. Chem. Phys. 145, 044310 (2016).

7. F. Kossoski, J. Kopyra, M. T. do N. Varella*. *Anion states and fragmentation of 2-chloroadenine upon low-energy electron collisions.* Phys. Chem. Chem. Phys. 17, 28958 (2015).

6. F. Kossoski, M. T. do N. Varella*. *Negative ion states of 5-bromouracil and 5-iodouracil.* Phys. Chem. Chem. Phys. 17, 17271 (2015).

5. J. Kopyra*, H. Abdoul-Carime, **F. Kossoski,** M. T. do N. Varella. *Electron driven reactions in sulphur containing analogues of uracil: the case of 2-thiouracil.* Phys. Chem. Chem. Phys. 16, 25054 (2014).

4. J. S. dos Santos, **F. Kossoski**, M. T. do N. Varella*. *Interaction of low-energy electrons with dimethyl sulfide and dimethyl disulfide.* Phys. Rev. A, 90, 052713 (2014).

3. F. Kossoski, M. H. F. Bettega, M. T. do N. Varella*. *Shape resonance spectra of uracil, 5-fluorouracil, and 5-chlorouracil.* J. Chem. Phys. 140, 024317 (2014).

2. F. Kossoski, M. H. F. Bettega*. *Low-energy electron scattering from the aza-derivatives of pyrrole, furan, and thiophene.* J. Chem. Phys. 138, 234311 (2013).

1. F. Kossoski, T. C. Freitas, M. H. F. Bettega*. *Resonances in electron collisions with $C_2H_2Cl_2$ isomers.* J. Phys. B: At. Mol. Opt. Phys. 44, 245201 (2011).

- **Publications in conference proceedings**

3. F. Kossoski*, M. Barbatti. *On-the-fly dynamics simulations of dissociative electron attachment to chloroethane.* J. Phys. Conf. Ser. 1412, 172010 (2020).

2. J. C. Ruivo*, **F. Kossoski**, M. T. do N. Varella*. *Investigation of electron scattering asymmetries in halocamphors.* J. Phys. Conf. Ser. 1412, 182018 (2020).

1. F. Kossoski, M. T. do N. Varella*. *Potential energy surfaces for anion states of 5-chlorouracil.* J. Phys. Conf. Ser. 635, 072086 (2015).

Invited and contributed talks in conferences

13. Invited talk: *State-specific configuration interaction for excited states*, in the Workshop on Excited-state Methods, Toulouse, France (2023).

12. Contributed talk: *Transient negative ions of a model radiosensitizer that do not undergo dissociative electron attachment and what it means for radiosensitivity,* in the Dynamics of Energetic & Electronic Processes in molecules and clusters in the GAS phase (DEEP-GAS), Madrid, Spain (2022).

11. Invited talk: *Emerging state-specific methods for electronic excitation*, in the 18th ETSF Young Researchers' Meeting, Marseille, France (2022).

10. Contributed talk: *A new route for electronic structure calculations: hierarchy configuration interaction***,** in the Les Rencontres des Chimistes Théoriciens Francophones, Bordeaux, France (2022).

9. Contributed talk: *Exploiting the seniority number in calculations of molecular excited states*, in the GDR Nbody General Meeting 2022, virtual (2022).

8. Invited talk: *Trajectory surface hopping dynamics of electronic resonances*, in the Workshop on Advances in Theory of Electronic Resonances, virtual (2021).

7. Invited talk: *On-the-fly nonadiabatic dynamics of electron-induced reactions*, in the Electron-Molecule Collisions and Swarms (EMS) – POSMOL, virtual (2021).

6. Invited talk: Trajectory surface hopping for nonadiabatic dynamics of resonances, in the Virtual International Seminar on Theoretical Advancements (VISTA), virtual (2021).

5. Contributed talk: *Multichannel coupling effects on electron collisions with ethanol*, in the Autumn Meeting of the Brazilian Physics Society, virtual (2021).

4. Invited talk: *Trajectory surface hopping dynamics for transient anions*, in the 2019 Conference on Light and Molecules, Marseille, France (2019).

3. Invited talk: *Direct dynamics simulation of electron-induced dissociation of chloroethane*, in the 7th Chinese-French Workshop in Theoretical Chemistry, Toulouse, France (2019).

2. Contributed talk: *Mechanisms of dissociative electron attachment to vinyl chloride*, in the 38th Brazilian National Meeting on Condensed Matter Physics, Foz do Iguaçu, Brazil (2015).

1. Contributed talk: *Bound and shape resonant anions of 5-bromouracil and 5-iodouracil*, in the 37th Brazilian National Meeting on Condensed Matter Physics, Costa do Sauípe, Brazil (2014).

Mentoring and teaching experience

- **Mentoring**

2021 – present	Yann Damour (PhD student)	Refs. 29, 35.
2020 – present	Alan G. Falkowski (PhD student)	Refs. 30, 34.
2019 – 2021	Julio C. Ruivo (PhD student)	Ref. 27.
2018 – 2020	Matheus B. Kiataki (PhD student)	Ref. 23.
2019 – 2020	Alan G. Falkowski (Master student)	Ref. 20.
2020	Leticia S. Maioli (PhD student)	Ref. 19.
2017	Lucas M. Cornetta (PhD student)	Ref. 10.
2014	Josué S. dos Santos (PhD student)	Ref. 4.

- **Teaching assistant**

2015 Physics I (undergraduate)
2014 Physics I (undergraduate)
2014 Introduction to Physics (undergraduate)
2013 Introduction to Atomic and Molecular Physics (undergraduate)
2013 Electricity and Magnetism I (undergraduate)
2012 Physics I (undergraduate)

Academic services

- **Event organization**

2023 Scientific organizing committee of the 19th ETSF Young Researchers' Meeting, Zaragoza, Spain.
2023 Local organizer of the Workshop on Excited-State Methods, Toulouse, France.

- **Peer reviewer**: 28 reports for 10 peer-reviewed scientific journals

Journal of Chemical Theory and Computation
Journal of Chemical Physics
Physical Chemistry Chemical Physics
International Journal of Molecular Sciences
Physical Review A
Physica Scripta
Journal of Physics B: Atomic, Molecular, and Optical Physics
The European Physical Journal D
European Journal of Physics
Journal of Physics: Conference Series

- **Jury member** in PhD and Master's defense and qualifying exams

2021 Jury member in the Master's qualifying exam (*suivi de thèse*) of Alan G. Falkowski, at Universidade Estadual de Campinas, Campinas, Brazil.

2021 Jury member in the PhD qualifying exam (*suivi de thèse*) of Letícia S. Maioli, at Universidade Federal do Paraná, Curitiba, Brazil.

2018 Jury member in the Master's dissertation of Matheus B. Kiataki, at Universidade Federal do Paraná, Curitiba, Brazil.

Languages

- English (fluent)
- French (intermediate)
- Spanish (intermediate)
- Portuguese (mother tongue)