Curriculum Vitae

Personal Information

Family name, first and middle names: Aucar, Ignacio Agustín
Researcher identifier: https://orcid.org/0000-0003-3501-0957
Date of birth and nationality: 02/07/1987, Argentine
Website: https://imit.conicet.gov.ar/en_aucar-i-agustin/
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Professional Profile

Experienced theoretical physicist with main interests in relativistic and QED effects in atomic and molecular properties

Education

- PhD in Physics, Northeastern University, Argentina
  Thesis topic: Effects of Heavy Atoms on Molecular Magnetic Parameters
  Advisor: Prof. Dr. Martín C. Ruiz de Azúa (University of Buenos Aires)
  Qualification and defense date: Outstanding with Special Mention, 18th December 2015
- Licentiate in Physical Sciences, Northeastern University, Argentina, 21th March 2011

Current and previous positions

01/03/2023 – 28/2/2025	Researcher 4, University of Groningen, Netherlands
2023 – present	Associate Researcher (on leave), National Research Council, Argentina
2015 – present	Assistant Professor (on leave), Northeastern University, Argentina
2021 – 2023	Associate Professor, Northeastern University, Argentina
2018 – 2023	Assistant Researcher, National Research Council, Argentina
2012 – 2015	Undergraduate Teaching Assistant, Northeastern University, Argentina
01/04/2016 – 31/10/2018	Postdoctoral Researcher at the IMIT Institute, Argentina

Publications (h-index: 7; total citations: 256; taken from Scopus, excluding self-citations)

Peer-reviewed Scientific Journals

†: corresponding author; blue text: master student under my co-supervision; []: number of citations

Data from Scopus, Sept. 2023

1. **I. A. Aucar**†, M. T. Colombo and G. A. Aucar, *A relativistic relationship between parity-violating nuclear spin-rotation tensors and parity-violating NMR shielding tensors*, J. Chem. Phys. **158**, 094306 (2023).
2. M. T. Colombo, K. Kozioł, **I. A. Aucar**, K. Gaul, R. Berger, and G. A. Aucar, *Relativistic and QED corrections to one-bond indirect nuclear spin-spin couplings in X_2^{2+} and X_3^{2+} ions (X = Zn, Cd, Hg)*, J. Chem. Phys. **157**, 064103 (2022).
3. **I. A. Aucar**†, Y. Chamorro and A. Borschevsky, *Parity-violating contributions to nuclear spin-rotation interactions and to NMR shielding constants in tetrahedral molecules*, Phys. Rev. A **106**, 062802 (2022).
4. **I. A. Aucar**† and A. Borschevsky, *Relativistic study of parity violating nuclear spin-rotation tensors*, J. Chem. Phys. **155**, 134307 (2021).
5. D. F. E. Bajac, **I. A. Aucar**, and G. A. Aucar, *Absolute NMR shielding scales in methyl halides obtained from experimental and calculated nuclear spin-rotation constants,* Phys. Rev. A **104**, 012805 (2021).
6. T. Saue, R. Bast, A. S. P. Gomes, H. J. Aa. Jensen, L. Visscher, **I. A. Aucar**, R. Di Remigio, K. G. Dyall, et al., *The DIRAC code for relativistic molecular calculations*, J. Chem. Phys. **152**, 204104 (2020).

7. K. Kozioł, **I. A. Aucar** and G. A. Aucar, *Relativistic and QED effects on NMR magnetic shielding constant of neutral and ionized atoms and diatomic molecules*, J. Chem. Phys. **150**, 184301 (2019).
8. **I. A. Aucar**†, C. A. Gimenez and G. A. Aucar. *Influence of the nuclear charge distribution and electron correlation effects on magnetic shieldings and spin-rotation tensors of linear molecules*, RSC Adv. **8**, 20234–20249 (2018).
9. G. A. Aucar, J. I. Melo, **I. A. Aucar** and A. F. Maldonado, *Foundations of the LRESC model for response properties and some applications*, Int. J. Quantum Chem. (**Review**) **118**, e25487 (2018).
10. **I. A. Aucar**, S. S. Gómez, C. G. Giribet and G. A. Aucar, *Role of Spin-Dependent Terms in the Relationship among Nuclear Spin-Rotation and NMR Magnetic Shielding Tensors*, J. Phys. Chem. Lett. **7**, 5188–5192 (2016).
11. **I. A. Aucar**, S. S. Gómez, C. G. Giribet and G. A. Aucar, *Toward an absolute NMR shielding scale using the spin-rotation tensor within a relativistic framework*, Phys. Chem. Chem. Phys. **18**, 23572 (2016).
12. **I. A. Aucar**, S. S. Gómez, C. G. Giribet and M. C. Ruiz de Azúa, *Theoretical study of the relativistic molecular rotational g-tensor*, J. Chem. Phys. **141**, 194103 (2014).
13. **I. A. Aucar**, S. S. Gómez, C. G. Giribet and M. C. Ruiz de Azúa, *Breit interaction effects in relativistic theory of the nuclear spin-rotation tensor*, J. Chem. Phys. **139**, 094112 (2013).
14. **I. A. Aucar**, S. S. Gómez, J. I. Melo, C. G. Giribet and M. C. Ruiz de Azúa, *Theoretical study of the nuclear spin-molecular rotation coupling for relativistic electrons and non-relativistic nuclei. II: Quantitative results in HX (X=H,F,Cl,Br,I) compounds*, J. Chem. Phys. **138**, 134107 (2013).
15. **I. A. Aucar**, S. S. Gómez, M. C. Ruiz de Azúa and C. G. Giribet, *Theoretical study of the nuclear spin-molecular rotation coupling for relativistic electrons and non-relativistic nuclei*, J. Chem. Phys. **136**, 204119 (2012).

Book Chapters

G. A. Aucar and **I. A. Aucar**, *Recent Developments in Absolute Shielding Scales for NMR Spectroscopy*, Annual Reports on NMR Spectroscopy. pp. 77-141. ISBN: 9780081028520. Graham A. Webb (editor). London, Academic Press (2019).

Teaching Activities

Courses taught as Associate Professor

- Thermodynamics (Physics degree, 1st year). *Lecturer.* 2023
- Experimental Physics I (Physics degree, 3rd year). *Lecturer.* 2021 and 2022
- General and Biological Physics (Biology degree, 1st year). *Lecturer.* 2021

Courses taught as (in charge) Assistant Professor

- Electricity and Magnetism (Physics degree, 2nd year). *Lecturer.* 2015 to 2022
- Optics and Sound (Physics degree, 2nd year). *Lecturer.* 2020
- Electricity, Magnetism, Optics and Sound (Chemistry degree, 3rd year). *Lecturer.* 2015, 2016, 2019
- Seminars of Modern Thermodynamics (Physics degree, 5th year). *Lecturer.* 2018
- Introduction to Relativistic Quantum Mechanics (Physics degree, 5th year). *Lecturer.* 2017 and 2022
- Classical Mechanics (Physics degree, 1st year). *Lecturer.* 2012, 2014 and 2015

Co-Lecturer in Post-graduate Courses

- Relativistic Quantum Physics. Applications to Atomic and Molecular Properties (PhD course). 2022
- Molecular Electronic Structure (PhD course). 2018
- Relativistic Effects in Molecular Magnetic Properties (PhD course). 2017

Grants

Current Grant				
Project Title	*Role*	*Funding source*	*Amount*	*Period (approx.)*
PICT-2020-SERIEA-00052 Study of Relativistic and parity non-conservation effects in nuclear spin-rotation constants. Application to heavy-elements containing molecular systems	Principal Researcher	Argentinean Agency for Promotion of Research, Technological Developments and Innovation (FONCyT)	AR$ 665,000 [equivalent to € 7,400, Jan. 2021]	July 2022 to June 2024
PIBAA 2022-2023 28720210100125CO Effects of relativity and parity violation on nuclear spin-rotation tensors	Principal Researcher	Argentinean National Scientific and Technical Research Council (CONICET)	AR$ 450,000 [equivalent to € 4,000, Jan. 2022]	November 2022 to October 2024

Supervision of Graduated Students

2023 Supervisor of the teaching training of a Junior Assistant Professor (Pablo F. Wagner-Boian). April 2022-April 2023. Northeastern University (UNNE), Argentina.

2020 Co-supervisor of a Master Student in Physics (Daniel F. E. Bajac), summa cum laude. Thesis title: "*Relativistic relationship between nuclear spin-rotation and NMR shielding tensors in non-linear heavy-element-containing molecules*". Defense: March 6th 2020. UNNE, Argentina

Oral Presentations in established Conferences and Meetings

- Authors: Ignacio Agustín Aucar, A. Borschevsky and Y. A. Chamorro Mena
  Title: *Parity violation effects on molecular properties: NMR shielding and nuclear spin-rotation constants in chiral molecules*
  Type of contribution: Invited Talk
  Congress: Physics Colloquium
  Organizing Institution: Fac. of Science and Engineering, Univ. of Groningen, The Netherlands
  Place and Year: University of Groningen, Groningen, The Netherlands, Oct. 2022
- Authors: Ignacio Agustín Aucar, D. F. E. Bajac and G. A. Aucar
  Title: *Absolute NMR shielding scales obtained from nuclear spin-rotation constants*
  Type of contribution: Invited Seminar
  Congress: Molecular Physics & Theoretical Chemistry Seminar Series
  Organizing Institution: Theoretical Chemistry Group, Univ. of Groningen, The Netherlands
  Place and Year: University of Groningen, Groningen, The Netherlands, Jun. 2022
- Authors: Ignacio Agustín Aucar, C. A. Gimenez and G. A. Aucar
  Title: *Influence of nuclear size and electron correlation effects on relativistic magnetic shielding and nuclear spin-rotation tensors*
  Type of contribution: Talk in the Atomic and Molecular Physics Division
  Congress: 103th Annual Meeting of the Argentine Physics Association
  Organizing Institution: Department of Physics, Univ. of Buenos Aires, Argentina
  Place and Year: University of Buenos Aires, Argentina, Sept. 2018
- Authors: Ignacio Agustín Aucar, S. S. Gomez, C. G. Giribet and M. C. Ruiz de Azúa
  Title: *Theoretical study of the relativistic rotational g-tensor*
  Type of contribution: **Invited Speaker**
  Congress: XI Relativistic Effects in Heavy-Element Chemistry and Physics International Conference
  Organizing Institution: Slovak Academic of Sciences, Bratislava, Slovak Republic
  Place and Year: Smolenice Castle, Bratislava, Slovak Republic, Sept. 2014

- Authors: Ignacio Agustín Aucar, S. S. Gomez and M. C. Ruiz de Azúa
  Title: *Molecular rotation effects over magnetic relativistic operators*
  Type of contribution: Invited Seminar
  Congress: Annual Meeting of the DIRAC code developers (workshop)
  Organizing Institution: DIRAC code developers
  Place and Year: Univ. of Southern Denmark, Odense, Denmark, Jun. 2014

Poster Presentations

- 10 Posters presented in Annual Meetings of the Argentinian Physics Society, between 2011 and 2021
- 1 Virtual poster presented at the LatinXChem Twitter Conference (2021)
- 1 Poster prepared for the 59th Sanibel Symposium, USA (2019)
- 4 Posters presented in the REHE International Conferences at Argentina (2012), Slovak Republic (2014), Germany (2017), and Italy (2022)
- 1 Poster prepared for the IX International Society for Theoretical Chemical Physics (ISTCP) Conference, USA (2016)
- 1 Poster presented at the European Summer-school on Quantum Chemistry, Italy (2013)
- 1 Poster prepared for the QUITEL Meeting (XXXVII Congress of Theoretical Chemists of Latin Expression), Mexico (2011)

Memberships of Scientific Societies

2008 – present Argentine Physics Society

Organisation of Scientific Meetings

2012 Member of the local organizing committee of the X Relativistic Effects in Heavy-Elements (REHE) International Conference. Corrientes (Argentina)

Fellowships and Awards

2023-2025 - Postdoc fellowship (24 months), University of Groningen (Netherlands)
Position: Researcher 4. Job profile: 01 08 40. Additional job profile: Post-doc.

2023 - Grant EINF-5787, SURF Cluster (Amsterdam) with 1,000,000 core hours of compute time

2022 - University of Groningen: short-stay visit of 11 weeks (Sep-Nov)
- HPC-Europa3 Project form the Horizon2020 Programme. Fellowship HPC17KOAX1
Visit of 13 weeks (Feb-Apr) to the University of Groningen (Netherlands)
- Grant EINF-3247, SURF Cluster (Amsterdam) with 1,000,000 core hours of compute time

2016-2018 - Postdoc fellowship (31 months), CONICET, Argentina

2014 - NEXT - Toulouse fellowship
Visit of 9 weeks (May-Jul) to the University Paul Sabatier, Toulouse (France)

2011-2015 - PhD fellowship (60 months), CONICET, Argentina

Reviewing Activities

Reviewer of "The Journal of Chemical Physics"
Member of an Exam Committee to Evaluate a Master Thesis in Physics, UNNE (2021)
Member of 2 Committees for the Recruitment of Assistant Professors in Physics, UNNE (2019 – 2022)
Member of 4 Committees for Periodic Evaluation of Assistant Professors in Physics, UNNE (2016 – 2021)

Software Development

- Developer of the *open-source* DIRAC code (http://diracprogram.org/ and https://gitlab.com/dirac/dirac) since 2013. This program computes molecular properties using relativistic quantum chemical methods.
  Main contributions/implementations: * Relativistic nuclear spin-rotation tensor (DIRAC-19.0).
  * Relativistic molecular rotational g-tensor (DIRAC-21.0).
  * Preliminary PV nuclear spin-rotation tensor (DIRAC-23.0).
  * Inclusion of CODATA sets of fundamental constants.
  * New entries for the manual, tutorial, and periodical updates.
- Contributor to the *open-source* EasyBuild program (https://easybuild.io). It is a build software that allows to managing (scientific) software on High Performance Computing (HPC) systems.
- Co-manager of the IMIT Institute's HPC cluster. Maintenance and installation of several scientific programs: DIRAC, DALTON, PySCF, QuantumEspresso, Wannier90, Gaussian, OpenFOAM, and others.

Public Outreach

2016 * Co-organizer and jury member of an annual competition for high-school students: "Measuring the acceleration of gravity". Invited Schools from the Provinces of Chaco and Corrientes, Argentina
* Presentation of an interactive experiment with lasers in the "Annual Week of Sciences", organized for primary- and high-school students. IMIT Institute, Corrientes, Argentina

2015 * Co-organizer and jury member of an annual competition for high-school students: "Using the light as a measuring instrument". Invited Schools from the Provinces of Chaco and Corrientes, Argentina
* Presentation of an interactive experiment with fluids in the "Annual Week of Sciences", organized for primary- and high-school students. IMIT Institute, Corrientes, Argentina

Relevant Attended Advanced Courses and Summer-Schools

- *Search for New Physics with Low-Energy Precision Tests Summer-School*. Ameland, Netherlands (2023), 56 hours
- *Spectroscopic Methods to Determine Molecular Structures*. Corrientes, Argentina (2014), 40 hours
- *Molecular Electronic Structure*. Corrientes, Argentina (2013), 90 hours
- *Computational Modeling and Simulation in Physics*. Corrientes, Argentina (2013), 90 hours
- *European Summer-school on Quantum Chemistry*. Sicily, Italy (2013), 2 weeks
- *Relativistic Quantum Chemistry and Molecular Physics*. Corrientes, Argentina (2012), 40 hours. Professors: Dr. S. Knetch (Denmark), Dr. K. Dyall (USA) and Dr. H. J. Aa. Jensen (Denmark)
- *Fundamentals of Quantum Electrodynamics and Applications to Atomic Systems*. Corrientes, Argentina (2012), 32 hours. Professors: Dr. J. R. Sapirstein (USA) and Dr. V. M. Shabaev (Russia)

Institutional Responsibilities

02/12/2021 – present Member of the (degree) Physics Degree Committee, UNNE, Argentina
27/10/2021 – present Member of the Academic Staff for the PhD in Physics, UNNE, Argentina