Joao Vitor Schober

Postdoctoral Researcher, University of Houston, TX, 77204

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Physical organic chemist with expertise in computational quantum chemistry (6+ years) and solution-state NMR spectroscopy (2+ years), complemented by data science in an industrial setting. Extensive collaborative experience with over five academic teams worldwide. Passionate about problem solving through computational modeling, analytical chemistry, and data science.

EDUCATION

Ph.D.	**Chemistry**	University of Houston, TX, USA	**2021 – 2025**
M.S.	**Chemistry**	University of Campinas – São Paulo, Brazil	**2019 – 2021**
B.S.	**Chemistry**	Federal University of Espirito Santo – ES, Brazil	**2015 – 2018**

SKILLS

- Programming skills: Python for data analysis, Scikit-Learn, NumPy, Pandas, Matplotlib, RDKit. Proficient in using Linux-based high-performance cluster for computational tasks.
- Nuclear Magnetic Resonance: Well versed in applying 1D and 2D NMR techniques, including HSQC, HMBC, TOCSY, NOESY, and DOSY. I am proficient in sample preparation, data acquisition, and processing using TopSpin and MNova. Strong understanding of the theoretical principles underlying NMR, demonstrated through 3 peer-reviewed publications.
- Computational chemistry: Extensive experience in electronic structure methods (e.g., ab initio, density functional theory, multireference methods) and software such as Gaussian, ORCA, Molpro, OpenMolcas, and Dalton. Proficient in diverse aspects of computational chemistry, such as structure optimization, reaction profiling, and modeling of excited states.
- Problem-solving & communication: Effective communicator with a strong track record of problem-solving across 5+ academic research teams worldwide. Collaborated with synthetic organic, inorganic, and analytical chemists while serving as the lead computational chemist on joint projects.

WORK & RESEARCH EXPERIENCE

Postdoctoral Researcher, University of Houston, TX, US (Cho Group). **Jan 2026 – Current**

- Developing a cheminformatics-driven, physics-informed screening pipeline to identify stable organic ground-state triplet molecules, combining graph-based molecular rules and quantum-chemical descriptors to accelerate discovery of new functional materials.

R&D Data Science Intern, Dow Inc. Core R&D Analytical Sciences, Lake Jackson, TX, US. **(Jun – Aug) 2025**

- Developed an approach to accelerate the acquisition of multidimensional NMR experiments for polymer analysis through machine learning, signal reconstruction techniques, and experimental NMR.
- Built a Python platform tool for processing and reconstruction of non-uniformly sampled NMR spectra, overcoming computational bottlenecks and enabling deployment on Dow's High-Performance Computing (HPC) systems.

Graduate Research Assistant, University of Houston, TX, US (Wu Group). **2021 – 2025**

- Developed a virtual screening method for the reactivity of aromatic compounds that is 200x faster than the traditional approach, allowing for high-throughput reactivity screening and reduced computational costs.
- Identified structure-property relationships influencing reactivity and stability of organic, organometallic, and photochemical systems by utilizing diverse electronic structure methods (i.e., DFT, CASSCF, and TD-DFT).
- I designed and directed two end-to-end research projects, taking full ownership from concept to dissemination as corresponding author on one publication (*Chem. Sci., 2024*) and another in preparation.
- Collaborated with 5+ research groups to address complex chemical problems in organic, inorganic, and theoretical chemistry, resulting in 5 publications, 3 talks, and 5 posters at national and international conferences.

Visiting Researcher, Uppsala University ,UP, Sweden (Ottosson Group). **(May – Jun) – 2024**

- Advanced the understanding of photochemical processes in aromatic molecules and photoacids using CASSCF and DFT simulations together with experimental measurements.

- Immersed in Sweden's sustainability culture, I gained a deeper appreciation for environmental responsibility, which prompted me to critically assess the carbon footprint of my own work. This reflection led me to begin tracking the emissions associated with my PhD research calculations.

Graduate Research Assistant, University of Campinas, SP, Brazil (Tormena Group) **2019 – 2021**

- Expanded knowledge of NMR coupling constants in fluorinated molecules—crucial for interpreting complex spectra—through synthesis, NMR spectroscopy, and computational chemistry, culminating in two peer-reviewed publications.

SELECTED HONORS AND AWARDS

- Jay K. Kochi Graduate Fellowship (1 out of 20). **2025**
- Best poster award at the 29th PHOTOIUPAC symposium | Valencia, Spain. **2024**
- Best poster award at 3rd ICESAA conference | Dubrovnik, Croatia. **2024**
- Poster award at 11th Young Researchers Conference | Texas A&M **2023**

LEADERSHIP AND OUTREACH

- Mentored underrepresented community college students in computational chemistry research, introducing them to molecular modeling, scripting, and data analysis. Helped develop individualized projects and guided students through scientific presentations.
- Co-organized an international research conference (2nd ICESAA) in Kauai, HI, coordinating sessions and supporting speaker logistics.

PUBLICATIONS (Google Scholar)

1. Phan, Son N.T.; **Schober, J.V.;** Wu, J.I.; Teets, T.S.* Synthesis and photoluminescence of iridium(iii) arylacetylide complexes with acetylide-localized emissive excited states. *Dalton Transactions,* **2026**. *Just accepted.*
2. Martins, F.; Viesser, R.V.; **Schober, J.V.**; Herges, R.;* Wu, J.I.* Triplet Spin Delocalization and Temperature Dependence for Adiabatic and Non-adiabatic Z-E Isomerization Pathways in Azoarenes. *J. Am. Chem. Soc.* **2025**, 147, 39, 35493–35500.
3. Dos Santos, N.R.; **Schober, J.V**.; Laconsay, C.J.; Kuhn, L.; Pallazo, A.; Hu, A.; Haddix, B.; Hanson, K.; Wu, J.I.*; Alabugin, I.V.* Assembly of pyrenes through a quadruple photochemical cascade: diversion from the double Mallory path to a new photocyclization at the bay region. *J. Am. Chem. Soc.* ***2025****, 147, 1, 1074–1091*.
4. **Schober, J. V**.*; Laconsay, C. J.; Wu, J. I.* Is Aromaticity Loss Obligatory for Transition-Metal Catalyzed Arene-Alkene Cycloadditions?. *Chem. Sci.* ***2024****, 15, 18093-18098*.
5. Karas, L. J.; Jalife, S.; Viesser, R. V.; **Soares, J. V.;** Haley, M. M.*; Wu, J. I.* Tetra-tert-butyl-s-indacence is a Bond Localized C2h Structure and a Challenge for Computational Chemistry. *Angew. Chem. Int. Ed.* **2023**, e202307379.
6. Nguyen, Y. H.;Dang, Q.V.; **Soares, J. V.;** Wu, J. I.; Teets, T. S.* Efficient blue-phosphorescent trans-bis (acyclic diaminocarbene) platinum(II) acetylide complexes. *Chem. Sci.* **2023**, 14, 4857-4862.
7. **Soares, J. V.**; Dal Poggetto, G.; Viesser, R. V.; Couto, U. R.; Tormena, C. F.* Stereoelectronic Interactions: A Booster for $^4J_{HF}$ Transmission. *Magn. Reson. Chem.* **2022**, 60, 481–488.
8. Nguyen, Y. H.; **Soares, J. V**.; Nguyen, S. H.; Wu, Y.; Wu, J. I.; Teets, T. S.* Platinum(II)-Substituted Phenylacetylide Complexes Supported by Acyclic Diaminocarbene Ligands. *Inorg. Chem.* **2022**, 61, 8498–8508.
9. Dal Poggetto, G.*; **Soares, J. V**.; Tormena, C. F. Selective Nuclear Magnetic Resonance Experiments for Sign-Sensitive Determination of Heteronuclear Couplings: Expanding the Analysis of Crude Reaction Mixtures. *Anal. Chem.* **2020**, 92, 14047–14053.
10. Maioli, J. P.; **Soares, J. V**.; Uliana, F.; Valim, T. C.; Francisco, C. S.; da Silva Filho, E. A.; Junior, V. L.; Neto, A. C.* Using NMR to Study the Process of Rigid Polyurethane Depolymerization. *Orbital: Electron. J. Chem.* **2019**, 11, 33–41.

Submitted/ In preparation

1. Hwang, J.†; Kim, H.†; **Schober, J. V.;** Gul Khan, M. U.; Barker, J. E.; Villarde, M. D.; Ni, X.; Wu, J. I.*; Gilliard, R. J., Jr.** Redox- and Protonation-Tunable Diboraheptacenes. *(In review on JACS)*.
2. **Schober, J. V.***; Ottosson, H.*; Wu, J.I.* Modulating Lewis interactions by excited-state aromaticity and antiaromaticity concepts. (*In preparation).*
3. Laconsay, C.J.; Dos Santos, N.R.; **Schober, J.V**.; Wu, J.I.*; Alabugin, I.V.* Photoinduced Azide Alkyne 1,3-Dipolar Cycloadditions Triggered by Excited-State Antiaromaticity Relief. (*In preparation).*