RYAN P. BRADY

PHD RESEARCHER – UCL

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Theoretical molecular spectroscopist with expertise in studying non-adiabatic interactions of complex diatomic systems. Key contributions include development of a novel method for the diabatisation of nuclear dynamics, production of a sulfur monoxide line lists utilized in JWST data, and producing research published in Nature, MNRAS, A&A, JCTC, and PCCP. Proven leadership in research coordination, international collaboration, conference presentations, chairing weekly research group meetings, and mentoring undergraduate students in cutting edge research projects.

SKILLS & ABILITIES

</> Python	Data Modelling/Analysis	</> HPC Experience
</> Julia	Mathematical Analysis	</> Linux, macOS
</> Fortran	Database Experience	Realisation of Theoretical Ideas
Mentoring/Teaching/Presenting	Fostering Scientific Partnerships	Self-Discipline and Goal Achievement

RESEARCH EXPERIENCE

PhD Research at ExoMol, Department of Physics & Astronomy, UCL (2021 - current)

- Investigation of non-adiabatic interactions for the nuclear dynamics of complex diatomic systems induced by non-Born-Oppenheimer and Spin-Orbit effects. Demonstration (for the first time) rovibronic equivalence of the adiabatic and diabatic representations and the importance of non-adiabatic couplings in rovibronic simulations.
- Development of an innovative methodology to compute a physical diabatic representation for diatomic nuclear dynamics, effectively regularizing non-adiabatic couplings to address inconsistencies from *ab initio* quantum chemistry calculations.
- Produced an accurate molecular line list for Sulfur Monoxide, successfully applied in multiple atmospheric retrievals of JWST exoplanet datasets.
- Successful fulfilment of research objectives ahead of grant timelines.
- Publishing of 10 scientific papers (3 first author) in peer-reviewed journals (Nature, MNRAS, A&A, PCCP, JCTC).
- Regular attendance and presenting of results at national and international meetings to promote my research and build collaborative networks.
- Chairman for ExoMol's weekly meetings, facilitating scientific discussions, and leading collaborative meetings with international scientists.

MSci Research at ExoMol, Department of Physics & Astronomy, UCL (2020 - 2021)

- Conducted a spectroscopic study on sulfur monoxide, producing an accurate empirical database of rotation-vibration energy levels with uncertainties and quantum number assignments.
- Collaborated internationally to perform high-level ab initio calculations which led to the development of a complex ab initio spectroscopic model aimed at improving high-temperature spectra modelling for exoplanetary atmospheres, addressing gaps in current spectroscopic databases.
- Solved coupled rovibronic Schrödinger equations to generate an *ab initio* line list for sulfur monoxide for 13 electronic states to which an *ab initio* IR/Vis/UV absorption spectra was computed over a wide range of temperatures.

Summer Research Internship with SNDUST, Department of Physics & Astronomy, UCL (2019)

- Studied dust formation in stellar outflows which included the modelling of H_α emission from supernovae 2004et.
- Results were included in a later publication to a peer-reviewed journal.

AWARDS

2021	**Tessela prize for best use of software in final (astro)physics master's project** Capgemini and the Department of Physics & Astronomy at UCL
2021	**Dean's list – The Faculty of Mathematical and Physical Sciences. Commends outstanding academic performance by graduating students, equivalent to the top 5% of student achievement.** Department of Physics & Astronomy at UCL
2019	**Huggins Prize for best performance in 2nd year astrophysics** Department of Physics & Astronomy at UCL

EDUCATION

2021 – Current	**PhD Research at ExoMol – Non-Adiabatic Interactions in Diatomic Molecules** Department of Physics & Astronomy at UCL
2017 – 2021	**1st Class MSci Astrophysics** Department of Physics & Astronomy at UCL
2017 – 2021	**A-Level Physics (A), Biology (A), Mathematics (A) / AS-Level Psychology (B)** Mayfield Grammar School

TEACHING EXPERIENCE

Orbyts mentor – outreach to empower school students to undertake world-leading research (ongoing)

- I have facilitated two research projects to A-level students at Parmiter's Secondary School, (1) Assignment of the Unstudied Spectra of Formaldehyde ($H2CO$) using a Detailed Quantum Mechanical Spectroscopic Model (2022), (2) Predissociation Broadening of Sulfur Monohydride (2023).
- Delivered lessons on basic quantum mechanics, its applications to molecular spectroscopy, and also data analysis using Python while teaching basis programming skills to students.
- Assisted students in designing and delivery of a research poster to be presented at the UCL Orbyts conference.

Mentor/Supervisor, Department of Physics & Astronomy, UCL (ongoing)

- Supervised and mentored multiple undergraduate students on diverse projects during my PhD, fostering their development in both theoretical and computational research.
- Provided support on projects including spectroscopic assignment, fitting of spectroscopic models to data, and advanced theoretical projects on non-adiabatic interactions.
- Assisted students with technical tasks such as setting up and using macOS systems and navigating high-performance computing (HPC) environments.

Mentor/Supervisor Physics Summer School, Department of Physics & Astronomy, UCL (2022)

- Designed and mentored a project for A-level students during the UCL physics summer school, focusing on spectral assignment of Formaldehyde.
- Developed a custom Python program for the project, guiding students through theory and coding.
- Provided mentorship on presentation skills and data plotting, culminating in the students delivering a final presentation to the entire summer school cohort.

ADDITIONAL SKILLS & COURSES

- Advanced Python Course (1 week; UCL; 2022)
- Fortran Course (1 week; UCL; 2022)
- DSD: Software for success: Data analysis & statistical tools (1 session; UCL; 2021)
- DSD: A Quick Introduction to UNIX (1 session; UCL; 2021)

PUBLICATIONS

[1] Tennyson, J.; Yurchenko, S. N.; Zhang, J.; Bowesman, C. A.; Brady, R. P.; Buldyreva, J.; Chubb, K. L.; Gamache, R. R.; Gorman, M. N.; Guest, E. R.; Hill, C.; Kefala, K.; Lynas-Gray, A.; Mellor, T. M.; McKemmish, L. K.; Mitev, G. B.; Mizus, I. I.; Owens, A.; Peng, Z.; Perri, A. N.; Pezzella, M.; Polyansky, O. L.; Qu, Q.; Semenov, M.; Smola, O.; Solokov, A.; Somogyi, W.; Upadhyay, A.; Wright, S. O.; Zobov, N. F. The 2024 release of the ExoMol database: Molecular line lists for exoplanet and other hot atmospheres. Journal of Quantitative Spectroscopy and Radiative Transfer 2024, 326, 109083.

[2] Brady, R. P.; Drury, C.; Yurchenko, S. N.; Tennyson, J. Numerical Equivalence of Diabatic and Adiabatic Representations in Diatomic Molecules. Journal of Chemical Theory and Computation 2024, 20, 2127–2139, PMID: 38171539.

[3] Buldyreva, J.; Brady, R. P.; Yurchenko, S. N.; Tennyson, J. Collisional broadening of molecular rovibronic lines. Journal of Quantitative Spectroscopy and Radiative Transfer 2024, 313, 108843.

[4] Powell, D.; Feinstein, A. D.; Lee, E. K. H.; et. al. Photochemically produced SO2 in the atmosphere of WASP-39b. Nature 2023, 617, 483–487.

[5] Brady, R. P.; Yurchenko, S. N.; Tennyson, J.; Kim, G.-S. ExoMol line lists – LVI. The SO line list, MARVEL analysis of experimental transition data and refinement of the spectroscopic model. Monthly Notices of the Royal Astronomical Society 2023, 527, 6675–6690.

[6] Liljegren, S.; Jerkstrand, A.; Barklem, P. S.; Nyman, G.; Brady, R.; Yurchenko, S. N. The molecular chemistry of Type Ibc supernovae and diagnostic potential with the James Webb Space Telescope. A&A 2023, 674, A184.

[7] Yurchenko, S. N.; Brady, R. P.; Tennyson, J.; Smirnov, A. N.; Vasilyev, O. A.; Solomonik, V. G. ExoMol line lists – LIII: empirical rovibronic spectra of yttrium oxide. Monthly Notices of the Royal Astronomical Society 2023, 527, 4899–4912.

[8] Brady, R. P.; Yurchenko, S. N.; Kim, G.-S.; Somogyi, W.; Tennyson, J. An ab initio study of the rovibronic spectrum of sulphur monoxide (SO): diabatic vs. adiabatic representation. Phys. Chem. Chem. Phys. 2022, 24, 24076–24088.

[9] Niculescu-Duvaz, M.; Barlow, M. J.; Bevan, A.; Wesson, R.; Milisavljeviç, D.; De Looze, I.; Clayton, G. C.; Krafton, K.; Matsuura, M.; Brady, R. Dust masses for a large sample of core-collapse supernovae from optical emission line asymmetries: dust formation on 30-year time-scales. Monthly Notices of the Royal Astronomical Society 2022, 515, 4302–4343.