**Asymmetric Organic Inorganic Hybrid Wells Dawson Polyoxometalates**

Noor Alnahdi, Kieran D. Jones, Graham N. Newton.

*GSK Carbon Neutral Laboratories for Sustainable Chemistry, Nottingham, UK*

noor.alnahdi@nottingham.ac.uk

Asymmetric organic-inorganic hybrid Wells Dawson polyoxometalates are phosphotungstates in which two different organic moieties are covalently bound to the cluster core.[1] The choice of the organic components plays a crucial role in tuning their electrochemical and physical properties.[2] By changing the organic component and bridging heteroatom (Sn, Si, P, As, etc), different functions and structural features can be achieved.

This poster describes the synthesis and characterisation of asymmetric hybrid polyoxometalates, bearing 3-phosphonopropionic acid (PPA) and 2,2':6',2''-terpyridine (TPY). The electro- and photo-chemical properties of these hybrid POMs were assessed by cyclic voltammetry and UV-Vis spectroscopy, respectively, and compared to those of the plenary parent POMs.

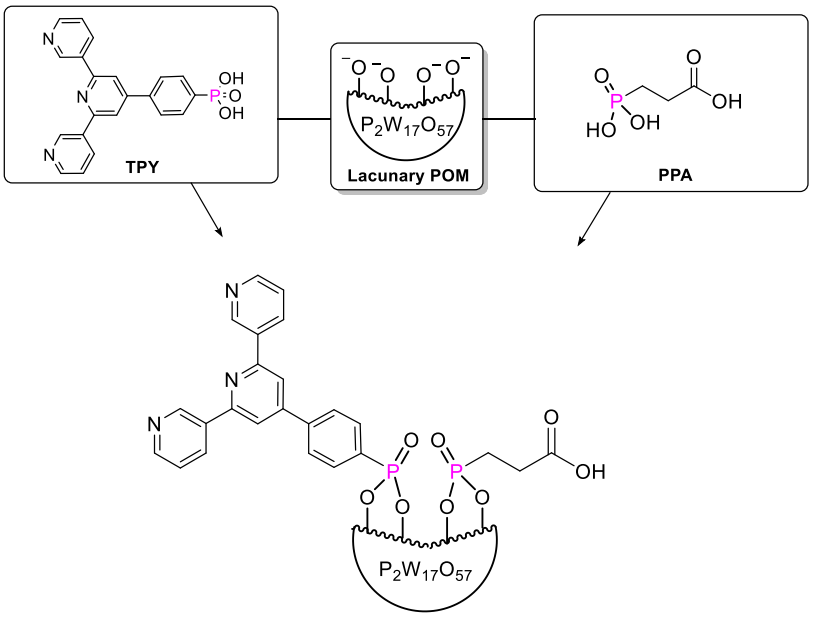



**Figure 1:** Synthesis of asymmetric hybrid polyoxometalates.

References

(1) Hampson, E.; Cameron, J. M.; Amin, S.; Kyo, J.; Watts, J. A.; Oshio, H.; Newton, G. N. Asymmetric Hybrid Polyoxometalates: A Platform for Multifunctional Redox-Active Nanomaterials. *Angew Chem Int Ed* **2019**, *58* (50), 18281–18285. https://doi.org/10.1002/anie.201912046.

(2) Martin, C.; Kastner, K.; Cameron, J. M.; Hampson, E.; Alves Fernandes, J.; Gibson, E. K.; Walsh, D. A.; Sans, V.; Newton, G. N. Redox-Active Hybrid Polyoxometalate-Stabilised Gold Nanoparticles. *Angew Chem Int Ed Engl* **2020**, *59* (34), 14331–14335. https://doi.org/10.1002/anie.202005629.

**Layered Lanthanum Oxyhalides For High-k Dielectric Materials**

Elizabeth L Hawkins[1*], Petros-Panagis Filippatos [1], Shayantan Chaudhury[1], Katherine Inzani[1]

1. *School of Chemistry, University of Nottingham*

*Presenting author: pcxeh2@exmail.nottingham.ac.uk

Silicon-based dielectrics are reaching scaling limits in semiconductor microelectronics. As transistors shrink to the atomic scale, quantum tunnelling and leakage currents become significant challenges, limiting further miniaturisation. New materials with superior properties are required to overcome this bottleneck.

Lanthanum oxyhalides (LaOX, X = F, Cl, Br, I) have recently been identified as promising materials due to their high dielectric constant (k), wide bandgap and chemical stability. As LaOX is a layered van der Waals material (vdW), they can retain these properties even at low dimensions.

This poster presents a density functional theory (DFT) based study of the structural, electronic, and dielectric properties of LaOX. Electronic properties are described using the HSE06 hybrid functional, while structural properties are modelled using r2SCAN+D3(BJ) MetaGGA. Ongoing work focuses on the effects of epitaxial strain as a method of tuning material properties for low-power electronic and quantum technology applications.

# Choice of Reduction Functions in Rainbow Tables

Mahfuzah Fariha[1]*, Xavier Carpent[1], Tim Muller[1]

1. *School of Computer Science, University of Nottingham*
*psymf9@nottingam.ac.uk

Rainbow tables, first introduced by Oechslin, are an example of a cryptanalytic Time-Memory Trade-Off technique used to address the pre-image problem, such as in the context of password recovery[1]. They offer a faster alternative to brute force attacks in recovering the pre-image of a one-way function, while reducing the memory required compared to utilising lookup tables. The process begins with the precomputation phase to explore the search space and store relevant values; followed by an online phase consisting of using these results for the attack itself.

Precomputation of rainbow tables involves creating chains of pre-images that make up the table itself[1]. However, due to collisions in the reduction function used in the process, many of these chains are discarded, resulting in a significant amount of wasted computation. Various techniques have been developed to improve the performance of the precomputation phase, such as introducing checkpoints to detect false alarms caused by the collisions[2], using different length chains[3], and recycling discarded chains[4], to name a few.

However, a previously overlooked area for improvement has been within the use of reduction functions. Usually, reduction functions are chosen arbitrarily, however the work introduced in this poster explores the extent of improvement cherry-picking reduction functions (a technique that selects the most effective reduction function from multiple candidates at each column position) brings rainbow tables in terms of coverage. Building upon preliminary work[5], we characterise how various parameters affect table density and performance. By improving these aspects, we can reduce the memory required to reach the same level of coverage of the search space, which, in turn, can improve upon the time needed to carry out the attack.

Our results demonstrate relationships between different table parameters, contributing to the characterisation of cherry-picking behaviour, and offering a foundation for alternative modelling strategies that reduce the added cost associated with incorporating cherry-picking. While our current model does not portray an accurate estimate of endpoints, the cherry-picking strategy it devises helps construct rainbow tables with significant improvement to a table's density.

1 P. Oechslin, in *Advances in Cryptology - CRYPTO 2003*, ed. D. Boneh, Springer, Berlin, Heidelberg, 2003, pp. 617–630.

2 G. Avoine, P. Junod and P. Oechslin, in *Proceedings of the 6th international conference on Cryptology in India*, Springer-Verlag, Berlin, Heidelberg, 2005, pp. 183–196.

3 G. Avoine and X. Carpent, in *Proceedings of the 2017 ACM on Asia Conference on Computer and Communications Security*, Association for Computing Machinery, New York, NY, USA, 2017, pp. 815–822.

4 G. Avoine, X. Carpent and D. Leblanc-Albarel, in *Proceedings of the 2023 ACM Asia Conference on Computer and Communications Security*, Association for Computing Machinery, New York, NY, USA, 2023, pp. 286–299.

5 S. K. Chandra, Masters Thesis, University of Nottingham, 2023.

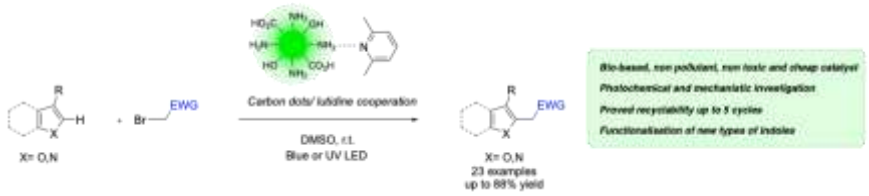
**Carbon nanodots as a new green nano-photocatalytic system for the C2-functionalization of indoles and heteroarenes derivatives**

M. Santoni[1*], J. Sargueil[2], S. Cichella[1], A. Di Sabato[1], F. Leonelli[1] and F. Vetica[1]

2. *Department of Chemistry, Sapienza University of Rome, Piazzale Aldo Moro 5, 00185 Rome, Italy*
3. *PPSM, Université Paris-Saclay, CNRS, ENS Paris-Saclay, Gif-Sur-Yvette 91190, France*

*marta.santoni@uniroma1.it

Carbon nanodots are a new class of carbon-based nanoparticles that are currently finding numerous applications in sensing, bio-imaging and heterogeneous catalysis, thanks to their easily tunable optical properties and superficial moieties. These versatile metal-free nanoparticles have been successfully employed in photocatalytic transformations as green and convenient replacements for the toxic, environmentally unsustainable and expensive transition metal complexes. [1-3] Herein, we report the application of carbon nanodots as a new green nano-photocatalytic system for the functionalization of indoles and heteroarenes derivatives to obtain 2-alkylated indoles, furanes and pyrroles in high yields (up to 88%). Moreover, this system is capable to access challenging entries such as indoles bearing electron-withdrawing groups on both carbon 2 (C2) and carbon 3 (C3). Photochemical and mechanistic studies consisting of Stern-Volmer analyses, fluorescence lifetimes, quantum yield and light-dark experiments were undertaken to gain additional insights on the reaction pathway. Furthermore, recyclability experiments proved the promising potential of these carbon nanodots as heterogenous and sustainable photocatalysts. Owing to their high photostability, this system presented photocatalytic activity up to 5 cycles without any significant loss in yield. [4]




**References**

[1] T. C. Wareing, P. Gentile and A. N. Phan, *ACS Nano* **2021**, 15, 10, 15471–15501, DOI: 10.1021/acsnano.1c03886

[2] M. Sbacchi, M. Mamone, L. Morbiato, P. Gobbo, G. Filippini, M. Prato, *ChemCatChem* **2023**, 15, e202300667, DOI: 10.1002/cctc.202300667;

[3] A. Di Sabato, M. Santoni, V. G. Moldoveanu, A. Camilli, M. Feroci, G. Olivo, B. Simonis, E. Sturabotti, F. Leonelli, F. Vetica, *Adv. Synth. Catal*. **2025**, 367, e202500354, DOI: 10.1002/adsc.202500354;

[4] J. Sargueil*, M. Santoni*, S. Cichella, A. Di Sabato, V. G. Moldoveanu, E. Sturabotti, B. Simonis, M. Giustini, L. M. Migneco, F. Leonelli and F. Vetica, *Chem. Eur. J.* **2025**, 31, e02043, DOI: 10.1002/chem.202502043.

# Investigating polymer-solvent interactions to assess solvation energy of polymers towards machine learning model development.

**Author (s):** Ronan Ozdural,[1,2,3] Daniel J. Keddie[1], Grazziela Figueredo[2], David Robinson[3], and Matt Addicoat [3]

1. School of Chemistry, University Park, Nottingham, Clifton Boulevard, NG7 2RD, United Kingdom

2. School of Medicine, Centre for Health Informatics, University Park, Nottingham, Clifton Boulevard, NG7 2RD, United Kingdom

3. School of Science and technology, Nottingham Trent University, Clifton Campus, Nottingham , Clifton Lane, NG11 8NS, United Kingdom

Author: ronan.ozdural@nottingham.ac.uk

**Abstract**

Polymer solutions are important for a wide range of applications including personal and home care formulations.[1] While machine learning (ML) has been used to predict bulk polymer properties, polymer properties in solution has been less studied. The polymer solvent system involves two interacting entities making prediction more challenging. Poly(acrylic acid) (PAA) is used here as a benchmark due to its extensive use in aqueous formulations for use as an viscosity modifier.[3] This makes it suitable for studying these polymer-solvent interactions.

Density functional theory (DFT) is employed to capture electronic and hydrogen-bonding effects for the polymer-solvent system. The PAA oligomer geometries are optimised at the ωB97X-D3/def2-TZVP level of theory, chosen for its reliable treatment of non-covalent interaction (see Figure 1). These DFT derived results and descriptors will form the foundation for developing a machine learning (ML) model.[3] Solvent effects are currently being explored using both implicit and explicit solvent models as part of ongoing work to understand their influence on PAA oligomer structure and solvation behaviour. This will be expanded upon in more complex 'real world' systems.

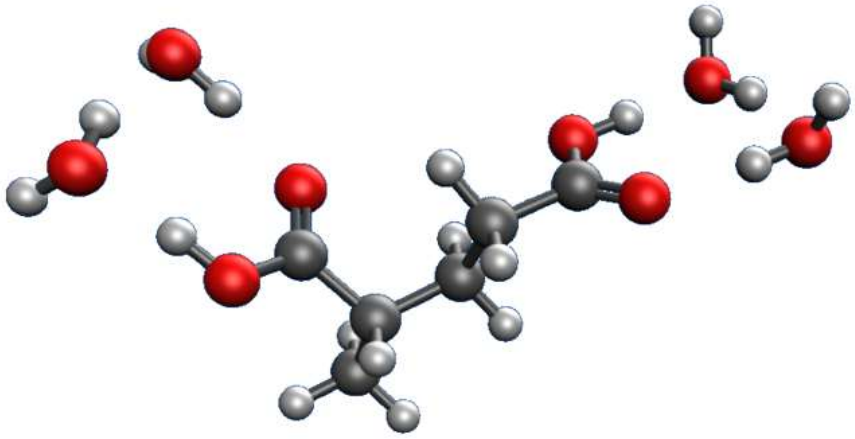


**Figure 1:** *Optimised geometry of PAA dimer with surrounding water molecules using* ωB97X-D3/def2-TZVP.

**References:**

*1. J. Nistane, L. Chen, Y. Lee, R. Lively and R. Ramprasad, MRS Communications, 2022, 12, 1096-1102.*

*2. Y. Aoki, S. Wu, T. Tsurimoto, Y. Hayashi, S. Minami, O. Tadamichi, K. Shiratori and R. Yoshida, Macromolecules, 2023, 56, 5446-5456.*

*3. J. Zhu, L.-H. Lin, H. Niu, Q. Shang, Q. Wang, F. Yan and J.-J. Li, Industrial & Engineering Chemistry Research, 2025, 64, 7862-7870.*

*4. Ł. M. Mentel and E. J. Baerends, Journal of Chemical Theory and Computation, 2014, 10, 252-267.*

**Ferroelectric $Hf_{1-x}Zr_xO_2$ Thin Films: A Materials Challenge for Machine-Learned Interatomic Potentials**

**Saffron Luxford**, Julie Greensmith, Valerio Giuffrida, Alex Ganose, Katherine Inzani

saffron.luxford@nottingham.ac.uk

Ferroelectric hafnia-based thin films have emerged as promising materials for nanoscale non-volatile memory and logic applications, combining ferroelectric behaviour with compatibility with silicon technology. Despite extensive experimental and theoretical effort, the microscopic origins of ferroelectricity in $Hf_{1-x}Zr_xO_2$ (HZO) remain incompletely understood. This is thought to be due to the complex interplay between composition, epitaxial strain, finite-size effects, interfacial chemistry, and defect formation, all of which influence the relative stability of closely competing polymorphs.

Density functional theory (DFT) has provided valuable atomistic insight into these mechanisms, but its high computational cost limits simulations to relatively small system sizes. As a result, many phenomena central to achieving reliable ferroelectricity thin-film devices, such as realistic heterointerfaces, extended defects, domain structures, and strain gradients, remain difficult to access directly. Machine-learned Force Fields (MLFFs) offer a promising route to bridge this gap, but their application to HZO poses significant challenges due to the material's narrow energy landscape, and sensitivity to charged defects.

In this work, we develop MACE-based interatomic potentials for HZO trained on VASP DFT configurations at the PBE level of theory. We demonstrate that MACE models accurately reproduce structural parameters from geometry optimizations, enabling rapid exploration of composition-strain-structure relationships.

Our work demonstrates the potential of machine-learned force fields to accelerate exploration of structure-property relationships in complex oxide ferroelectrics, providing a pathway to computational screening at scales beyond the reach of conventional DFT while targeting quantitative accuracy for both structural and electronic descriptors.

## XX Acceptorless alcohol dehydrogenation using sulfur-based manganese catalysts

**Isabelle Marriott**,[a] , Jonathan McMaster,[b] Deborah Kays,[c] Peter Licence[a]

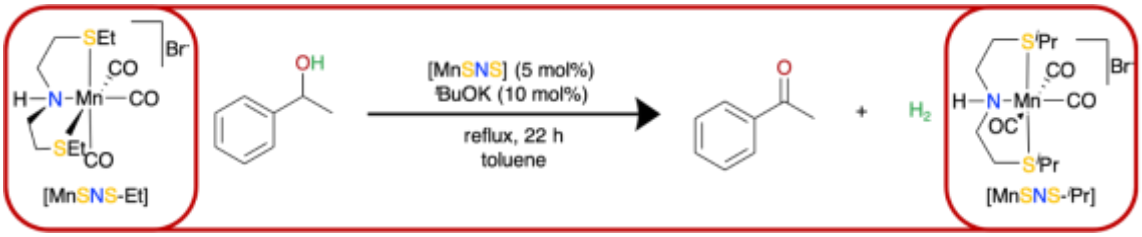
[a] GSK Carbon Neutral Laboratories, University of Nottingham, Jubilee Campus, Nottingham, NG7 2GA [b] School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD [c] School of Chemistry, Cardiff University, Cardiff, CF10 3AT

E-mail: isabelle.marriott@nottingham.ac.uk

Reversable carbonyl formation from alcohols *via* Acceptorless alcohol dehydrogenation (AAD) have shown promise as a hydrogen storage medium for use as an energy vector.[1] This chemistry has long been dominated by noble metals, particularly ruthenium, osmium and iridium,[1] which raises questions over these catalysts sustainability. Whilst advances have been made with base metal AAD catalysts, notably iron, manganese and cobalt,[2] these advancements often utilize phosphorus-based ligand systems which can be synthetically difficult to work due their air sensitive nature.

As such sulfur-based ligand systems are a rational alternative due to their air stability and their relative ease of use. Building on work by Schörgenhumer *et. al.* with ruthenium-sulfur AAD catalysts[3] and manganese-sulfur hydrogenation catalysts by Grover *et. al,*[4] herein we present a manganese-sulfur catalyst capable of performing AAD reactions.

From our initial results, the effect of ligand lability has on AAD reactions as well as any impact of complex geometry and electronics can be explored.




Reaction scheme for manganese-catalysed AAD reaction using sulfur-based ligand systems.

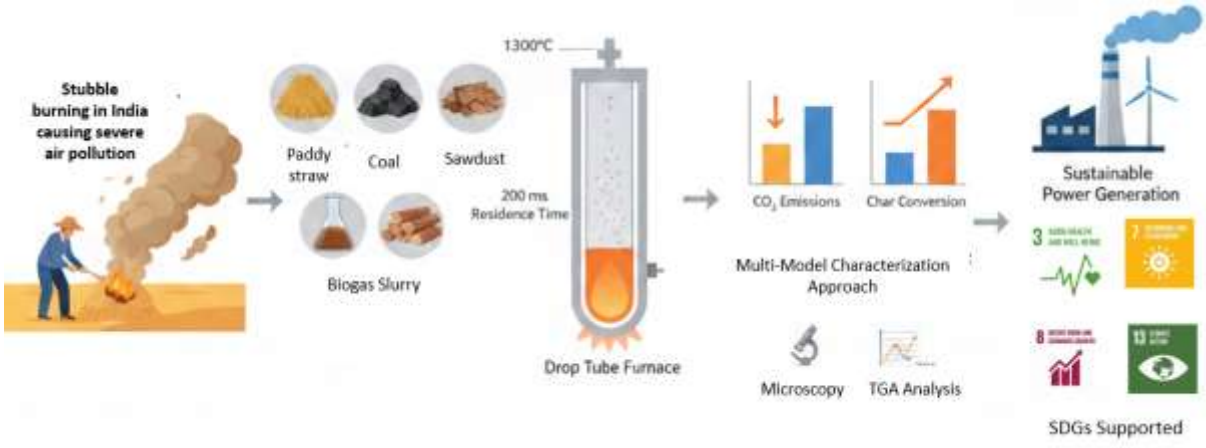
References

1. J. Campos, *Phys. Sci. Rev.*, 2018, **3**, 1–40.
2. M. Trincado, J. Bösken and H. Grützmacher, *Coord. Chem. Rev.*, 2021, **443**, 213967.
3. J. Schörgenhumer, A. Zimmermann and M. Waser, *Org. Process Res. Dev.*, 2018, **22**, 862–870.
4. J. Grover, S. Maji, C. Teja, S. A. Al Thabaiti, M. M. M. Mostafa, G. K. Lahiri and D. Maiti, *ACS Org. Inorg. Au*, 2023, **3**, 299–304.

**Combustion for Clean Air: Co-Firing Rice Paddy Residue with Coal to Eliminate Paddy field Burning and Reduce Power-Sector Emissions in India**

Deepti[1,2,3*], Orla Williams[2], Ed Lester[2], Kunwar Pal[3], Nikhil Gakkhar[4], Amrit Pal Toor[1]

[1]*Dr. SSBUICET, Panjab University, Chandigarh, India 160014*
[2]*Advanced Materials Research Group, Faculty of Engineering, University of Nottingham, Nottingham, United Kingdom, NG7 2DU*
[3]*Thermo-Chemical Division, Sardar Swaran Singh National Institute of Bioenergy, Kapurthala, Punjab, India 144603*
[4]*Ministry of New and Renewable Energy, New Delhi, India, 110003*
[*]*Corresponding author: Deepti.deepti@nottingham.ac.uk*




**Abstract:** Open-field burning of rice residue is a major seasonal source of particulate pollution in northern India, severely degrading air quality. Redirecting this residue into controlled combustion processes eliminates those field-burning emissions while utilising an otherwise wasted biomass resource. Co-firing this biomass with coal also lowers the overall carbon intensity of power generation, supporting India's wider transition toward cleaner energy. This Commonwealth Split-Scholarship project between India's Punjab University and the University of Nottingham uses UK expertise and facilities to accelerate India's transition by providing access to advanced combustion and analytical equipment not currently available in India.

This study aims to explore the potential of co-firing of paddy straw (sourced from the major paddy-producing states of Haryana and Punjab) and coal in pulverised fuel (PF) systems for power generation. The study conducted simulated PF combustion trials using a Drop Tube Furnace at 1300°C, with a residence time of 200 ms. Three particle sizes were tested (53-75 µm, 125-150 µm and 212-300 µm) for paddy straw, Indian coals, and two binders, a biogas slurry and sawdust. Tests were conducted at 20, 40, 60 and 80% blend ratios, and chars were collected. $CO_2$ emissions were recorded during test, and particulate matter was collected for further analysis. The coals and biomasses were characterised before and after combustion using a range of comprehensive tests including petrographic analysis, thermogravimetric analysis, particle size and shape analysis using a CamSizer, helium pycnometry and elemental analysis. The novelty lies in assessing coal–paddy–binder interactions under PF-relevant conditions and applying a multi-modal characterisation approach that provides rare insight into combustion-to-char

transformations of agricultural residues, while generating data that will guide forthcoming pelletised-fuel testing in India.

This research promotes the use of agricultural residues as a sustainable alternative to open-field burning, reducing environmental harm and health risks in line with SDG 3 (Good Health and Well-being) and SDG 13 (Climate Action). Beyond the combustion benefits, it supports rural livelihoods by creating jobs in biomass collection, processing and densification, contributing to SDG 8 (Decent Work and Economic Growth). The findings also provide valuable evidence to support national policies—such as India's mandate for 20% biomass co-firing—offering a practical pathway toward SDG 7 (Affordable and Clean Energy) through scalable, low-carbon power generation.

**Keywords:** Composite fuels, Co-Combustion, coal, paddy straw, emissions reduction, net zero energy

**Acknowledgement:** The author gratefully acknowledges the Commonwealth Scholarship Commission (CSC), United Kingdom, for funding this research through the Commonwealth Split-Site PhD Scholarship, supported by the UK Foreign, Commonwealth & Development Office (FCDO).

**Investigating binding partners of the N-terminal domain of HelQ using multi-dimensional NMR**

Alice Nottingham[1*], Panos Soultanas[1], Ed Bolt[2], Huw Williams[1]

1. *School of Chemistry, Biodiscovery Institute, University of Nottingham NG7 2RD*
2. *School of Life Sciences, University of Nottingham NG7 2RD*

*Presenting author: mbyan4@nottingham.ac.uk

Ovarian cancer is the most fatal gynaecological malignancy, with a mortality rate of over 200,000 per year[1]. The DNA repair helicase HelQ has been implicated in ovarian cancer, with previous experiments identifying a strong correlation between HelQ expression and patient prognosis[2].

HelQ has been linked to a number of DNA repair pathways, especially those involved in the repair of double-stranded DNA breaks, but its exact role in these pathways is currently unknown. Recent research from the University of Nottingham has identified the N-terminal region of HelQ (N-HelQ) as a site of protein-protein interactions due to its intrinsically disordered nature, providing insight into the helicase's role within repair[3].

This study aims to examine how intrinsic disorder influences the role of N-HelQ in DNA repair and investigate these potential interactions through multi-dimensional NMR spectroscopy. We propose that N-HelQ acts as a hub protein and plays a critical role in facilitating double-strand DNA break repair by homologous recombination. We present data investigating N-HelQ, its structure and its interactions with the proposed binding partners Polymerase δ and Replication Protein A[4].

References

(1) Tan, S.; Zhu, F.; Li, Y.; Wen, X.; Yang, S.; Liao, Z.; Duan, X.; Xiao, D.; Zhang, Y. *Translational Oncology* **2025**, *57* (102416), 11.

(2) Long, J.; Zhu, J.-Y.; Liu, Y.-B.; Fu, K.; Tian, Y.; Li, P.-Y.; Yang, W.-Q.; Yang, S.-Y.; Yin, J.-Y.; Yin, G.; et al. *Gynecological Oncology* **2018**, *149*, 341-349.

(3) Jenkins, T.; Northall, S. J.; Ptchelkine, D.; Lever, R.; Cubbon, A.; Betts, H.; Taresco, V.; Cooper, C. D. O.; McHugh, P. J.; Soultanas, P.; et al. *Nucleic Acids Research Cancer* **2021**, *3* (1).

(4) He, L.; Lever, R.; Cubbon, A.; Tehseen, M.; Jenkins, T.; Nottingham, A. O.; Horton, A.; Betts, H.; Fisher, M.; Hamdan, S. M.; et al. *Nucleic Acids Research* **2023**, *51* (4), 1740-1749.

# A Radio Frequency Interference Detection and Analytical Geolocation Method Demonstrated from LEO with an End-To-End Simulator and Cyclone GNSS Raw Data

T. Yousif[1*], P.Blunt[1], P.Christopher[1]

[1]*Nottingham Geospatial Institute Research Group, College of Engineering, University of Nottingham, Nottingham*

*tasneem.yousif@nottingham.ac.uk

Global Navigation Satellite Systems (GNSS) receivers are used worldwide in a wide range of applications, including military operations, precision agriculture, spaceborne missions, timing synchronisation, aviation, maritime navigation, and ground transportation. However, GNSS receivers operate on extremely weak signals (typically ≤ 160 dBW) and are therefore vulnerable to many forms of interference[1, 2]. With the growing incidence of GNSS disruption in the current geopolitical climate, radio-frequency interference (RFI) has become one of the major challenges facing GNSS users, as it can introduce significant errors in signal reception and degrade the accuracy and reliability of GNSS-based positioning, navigation, and timing (PNT). For space applications, characterising and mapping RFI is particularly challenging because large free-space path losses further weaken the received signals. Consequently, detecting and localising RFI from satellites is a highly desirable capability for applications such as GNSS-Reflectometry, search-and-rescue, surveying, and spectrum monitoring.

This research presents an analytical method based on the Doppler shift and Doppler rate measurements using a single Low Earth Orbit (LEO) satellite to detect and geolocate RFI transmitters. The methods are demonstrated using RFI-simulated data generated with the Orolia Skydel GNSS simulator and validated against historical Cyclone GNSS (CYGNSS) raw data. The geolocation method provides an unambiguous, converged, and stable solution through an optimisation process that estimates the location of the RFI transmitter. The RFI detection method is based on the short-time Fourier transform (STFT), which is robust in low signal-to-noise ratio (SNR) environments, operating reliably down to –35 dB. The geolocation method is computationally efficient, operating on short data windows (30–60 seconds) and accommodating different types of interference. Two CYGNSS raw IF datasets were selected for detection and geolocation. The geolocation algorithm produced a converged and consistent estimated RFI transmitters at the global minimum of the cost function, while also providing accurate vertical positioning of the RFI sources through the use of the Copernicus GLO-30 Digital Elevation Model (DEM). The geolocation accuracy for the simulated RFI scenarios was approximately within (20–50) meters, while for overhead scenarios it was 800 meters, reflecting the sensitivity of the analytical model that has been addressed in this project. The end-to-end simulation allows assessments of the accuracy in a variety of scenarios, while the CYGNSS raw data demonstrate the method and techniques applied to current in-orbit data.

This work makes a significant contribution to the characterisation and mapping of GNSS interference for space applications. It also assesses the complexity of different interference scenarios in terms of type (continuous-wave jammer, sweeping-jammer, and spoofing), power level, and the number of simultaneous interferers. Unlike existing studies[3], this research is the first to utilise CYGNSS raw intermediate-frequency (IF) data channels for RFI detection and geolocation. Furthermore, Monte Carlo simulations are conducted to evaluate the robustness of the proposed approach and its sensitivity to key factors affecting geolocation accuracy, including the inflection-point time, transmitter height, and transmitter clock offset.

[1] T. Yousif and P. Blunt, "Interference mitigation for GNSS receivers using FFT excision filtering implemented on an FPGA," *Eng,* vol. 3, no. 4, pp. 439-466, 2022.

[2] T. Yousif, B. Wadsworth, P. Christopher, and P. Blunt, "A novel GNSS RF interference detection and geolocation algorithm for LEO satellites," in *Proceedings of the 37th International Technical Meeting of the Satellite Division of The Institute of Navigation (ION GNSS+ 2024)*, 2024, pp. 3375-3389.

[3] C. Chew, T. M. Roberts, and S. Lowe, "RFI Mapped by Spaceborne GNSS-R Data," *NAVIGATION: Journal of the Institute of Navigation,* vol. 70, no. 4, 2023.

**Understanding and Encouraging Voice Interaction in Driving: Barriers, Motivation, and Digital Nudging**

Sparsh Khandeparker*, Catherine Harvey, David R. Large

3. *School of Engineering, University of Nottingham*

sparsh.khandeparker@nottingham.ac.uk

Voice interaction enables drivers to operate in-vehicle systems hands-free and eyes-free, supporting visual attention to the road and offering safety advantages over visual–manual interfaces (McLean & Osei-Frimpong, 2019). Despite this, in-vehicle voice systems are not used to their potential and are typically limited to simple tasks (Lee & Jeon, 2022). Recent advances in Artificial Intelligence (AI) have expanded voice assistant capabilities (Huang et al., 2024), highlighting the need to understand barriers to their use in driving and how these may be addressed. This PhD therefore investigates why drivers do not fully use in-car voice systems and explores strategies to encourage its use.

The research began with a literature review examining the evolution of voice systems (dialogue systems) and the role of AI in shaping their capabilities. Early voice systems were command-driven with restricted vocabularies, whereas conversational dialogue systems (conversational AI or voice assistants/agents) eliminated the need for predefined commands, improving usability (Gusikhin et al., 2007; Luger & Sellen, 2016). The integration of large language models has further expanded contextual understanding and generative capacity in domain-specific applications (Feuerriegel et al., 2024).

Building on this, an interview study explored user perceptions across home and driving contexts. Inductive thematic analysis identified eight factors influencing use, including performance, privacy, prior experience, perceived effort, user preference, system dormancy, multiple agents, and perceived loss of authority. These insights informed a large-scale survey. Seventy items were refined through exploratory and confirmatory factor analyses across two rounds of data collection (N = 511), resulting in a 19-item scale with three core factors: system performance, privacy, and system utility. Contrary to expectations, privacy was not perceived as a major barrier. Utility was rated as important, while perceptions of performance were largely neutral. Further analysis indicated that drivers feel confident using voice systems but lack motivation to do so.

To address this motivational gap, nudge theory (Thaler & Sunstein, 2008) was adopted. As prior research had not applied nudging to in-vehicle voice interaction, this study addressed a novel gap. Drawing on dual-process theory(Krämer, 2014), Fogg's Behaviour Model(Fogg, 2009), and empirical findings, six strategies were selected from the 23 proposed by (Caraban et al., 2019): priming, reciprocity, scarcity, inferior alternatives, placebos, and biasing memory. An exploratory study with eight experts in human factors, voice interaction, and driving evaluated their suitability. Deductive thematic analysis identified promising nudges (priming, inferior alternatives), problematic ones (reciprocity, scarcity), and those with low salience (placebos, biasing memory), alongside design recommendations. These findings inform a simulator-based study implementing the most promising nudges in a functional in-vehicle prototype to examine behavioural impact and safety implications, moving beyond perceived effectiveness toward real-world applicability.

Caraban, A., Karapanos, E., Gonçalves, D., & Campos, P. (2019). 23 Ways to Nudge: A review of technology-mediated nudging in human-computer interaction. *Conference on Human Factors in Computing Systems - Proceedings*. https://doi.org/10.1145/3290605.3300733

Dittrich, M., Ko, S., & Rieger, T. (2025). Impact of Voice Assistants' Conversational Style on Cognitive Driver Distraction. *IVA 2025 - Proceedings of the 25th ACM International Conference on Intelligent Virtual Agents*. https://doi.org/10.1145/3717511.3749294

Feuerriegel, S., Hartmann, J., Janiesch, C., & Zschech, P. (2024). Generative AI. *Business and Information Systems Engineering*, *66*(1), 111–126. https://doi.org/10.1007/s12599-023-00834-7

Fogg, B. (2009). A behavior model for persuasive design. *ACM International Conference Proceeding Series*, *350*. https://doi.org/10.1145/1541948.1541999;WGROUP:STRING:ACM

Gusikhin, O., Rychtyckyj, N., & Filev, D. (2007). Intelligent systems in the automotive industry: Applications and trends. In *Knowledge and Information Systems* (Vol. 12, Number 2). https://doi.org/10.1007/s10115-006-0063-1

Huang, S., Zhao, X., Wei, D., Song, X., & Sun, Y. (2024, May 11). Chatbot and Fatigued Driver: Exploring the Use of LLM-Based Voice Assistants for Driving Fatigue. *Conference on Human Factors in Computing Systems - Proceedings*. https://doi.org/10.1145/3613905.3651031

Krämer, W. (2014). Kahneman, D. (2011): Thinking, Fast and Slow. *Statistical Papers*, *55*(3), 915–915. https://doi.org/10.1007/S00362-013-0533-Y

Lee, S. C., & Jeon, M. (2022). A systematic review of functions and design features of in-vehicle agents. *International Journal of Human-Computer Studies*, *165*, 102864. https://doi.org/10.1016/J.IJHCS.2022.102864

Luger, E., & Sellen, A. (2016). "Like having a really bad pa": The gulf between user expectation and experience of conversational agents. *Conference on Human Factors in Computing Systems - Proceedings*. https://doi.org/10.1145/2858036.2858288

McLean, G., & Osei-Frimpong, K. (2019). Hey Alexa … examine the variables influencing the use of artificial intelligent in-home voice assistants. *Computers in Human Behavior*, *99*. https://doi.org/10.1016/j.chb.2019.05.009

Shin, J., Ko, H., Bae, S. W., & Kim, J. (2025). An Exploratory Study on the Impacts of Voice-Based Conversational Agents with Proactive Interactions in the Driving Context. *International Journal of Human-Computer Interaction*, *41*(6). https://doi.org/10.1080/10447318.2024.2441530

Thaler, R. H., & Sunstein, C. R. (2008). Nudge: Improving decisions about health, wealth, and happiness. In *Nudge: Improving Decisions about Health, Wealth, and Happiness*. https://doi.org/10.1016/s1477-3880(15)30073-6