Harry W. T. Morgan

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Education

University College, University of Oxford — *Oxford, UK*

Theory and Modelling in Chemical Sciences CDT (TMCS) — *2017-2021*

- **MSc Theoretical and Computational Chemistry** — *2017-2018*
- **DPhil Computational Inorganic Chemistry**, — *2018-2021*

New College, University of Oxford — *Oxford, UK*

MChem Chemistry, First Class honours — *2013-2017*

Trinity College London — *Bristol, UK*

ATCL Diploma in Recorder Performance, Distinction — *2013*

Clifton College — *Bristol, UK*

School education — *2007-2012*

- **A levels** — Chemistry, Physics, Maths, Further Maths - A*; Classical Greek - B
- **GCSEs** — English Literature, English Language, Mathematics, Biology, Chemistry, Physics, History, French, Latin, Classical Greek, Religious Studies – A*
- **ABRSM Grade 8 Practical Music** — Recorder, 'Cello, Piano

Key skills and achievements

Academic scholarships	Radcliffe scholarship to University College, Undergraduate academic scholarship at New College
Research leadership	Independently planned, managed and completed a collaborative research project
Undergraduate teaching	Devised and taught inorganic chemistry tutorials and quantum supplementary classes
Graduate supervision	Supervised masters' projects and taught computational methods to new graduate students
Scientific writing	Wrote scientific journal articles and a weekly food chemistry blog
Research presentation	Gave talks at national RSC conferences and Oxford departmental seminars
Peer review	Independent reviewing activity for international chemistry journals
Undergraduate admissions	Assisted with all stages of the undergraduate admissions process at New College, Oxford

Experience

University of California, Los Angeles — *Los Angeles, California, USA*

Postdoctoral Scholar — *Oct. 2021 - present*

- Research on the electronic structure of fluxional sub-nano clusters at heterogeneous catalyic interfaces

Magdalen College, Oxford — *University of Oxford, UK*

Lecturer — *Oct. 2020 - Oct. 2021*

- Jointly responsible of the inorganic chemistry teaching to 20-30 undergraduate students across all three years of the course
- Prepared and delivered three hours of tutorials per week alongside classes and assessments

New College, Oxford — *University of Oxford, UK*

Graduate Teaching Assistant, undergraduate admissions interviewer — *Oct. 2018 - Oct. 2021*

- Prepared and taught weekly classes to second year chemists taking the quantum chemistry supplementary course and additional classes in inorganic chemistry
- Conducted undergraduate admissions interviews in inorganic chemistry and contributed to final decisions

Projects

Metal-metal bonding in periodic transition metal systems *University of Oxford*

DPhil project with Prof. John McGrady *Oct. 2018 - present*

- Symmetry and structure in group 14 endohedral clusters - trends in complex cluster families by orbital analysis and fragment assembly, and encapsulation of paramagnetic atoms
- Structural processes in perovskite oxyhydrides - using static calculations alongside experiments and dynamic simulations to explore high-pressure transitions and ionic conduction mechanisms, and predict new materials
- Bonding in MoS_2 monolayer systems with adsorbed transition metal atoms - addressing challenging single atom catalysts by combining periodic DFT, including local projection methods, with molecular DFT and CASSCF

Structural and electronic properties of perovskites and reduced derivatives *University of Oxford*

Part II project with Prof. John McGrady *Sep. 2016 - July 2017*

- Studied electronic factors in the structural preferences of $A_2B_2O_5$ brownmillerites
- Learned to perform and analyse periodic DFT calculations in VASP
- Investigated metal-metal interactions and the role of spin-orbit coupling in 3d/5d double perovskites

Publications

Open Shells in Endohedral Clusters: Structure and Bonding in the $[Fe_2@Ge_{16}]^{4-}$ Anion and Comparison to Isostructural $[Co_2@Ge_{16}]^{4-}$
H. W. T. Morgan, K.-S. Csizi, Y.-S. Huang, Z.-M. Sun, and J. E. McGrady *Journal of Physical Chemistry A*, 125 (2021) 21, 4578–4588, 10.1021/acs.jpca.1c02837

Improving Hydride Conductivity in Layered Perovskites via Crystal Engineering
H. W. T. Morgan, H. J. Stroud, and N. L. Allan
Chemistry of Materials, 33 (2021), 1, 177, 10.1021/acs.chemmater.0c03177

$[Cu_4@E_{18}]^{4-}$ (E = Sn, Pb): Fused Derivatives of Endohedral Stannaspherene and Plumbaspherene
L. Qiao, C. Zhang, C.-C. Shu, **H. W. T. Morgan**, J. E. McGrady, and Z.-M. Sun
Journal of the American Chemical Society, 142 (2020) 13288-13293, 10.1021/jacs.0c04815

A family of lead clusters with precious metal cores
C.-C. Shu, **H. W. T. Morgan**, L. Qiao, Z.-M. Sun and J. E. McGrady
Nature Communications, 11 (2020) 3477, 10.1038/s41467-020-17187-4

Pressure-induced transitions in 1-dimensional vanadium oxyhydrides Sr_2VO_3H and $Sr_3V_2O_5H_2$ and comparison to 2-dimensional $SrVO_2H$
T. Yamamoto, **H. W. T. Morgan**, D. Zeng, T. Kawakami, M. Amano Patino, M. A. Hayward, H. Kageyama, J. E. McGrady
Inorganic Chemistry, 59 (2019) 15393, 10.1021/acs.inorgchem.9b02459

Structural isomerism in the $[(Ni@Sn_9)In(Ni@Sn_9)]^{5-}$ Zintl ion
C. Zhang, **H. W. T. Morgan**, Z.-C. Wang, C. Liu, Z.-M. Sun, and J. E. McGrady
Dalton Transactions, 48 (2019) 15888, 10.1039/C9DT03008E

Sr_2FeIrO_4: Square-Planar Ir(II) in an Extended Oxide
J. E. Page, **H. W. T. Morgan**, D. Zeng, P. Manuel, J. E. McGrady and M. A. Hayward
Inorganic Chemistry, 57 (2018) 13577, 10.1021/acs.inorgchem.8b02198

References

Prof. John McGrady
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Prof. Neil Allan
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neil.allan@bristol.ac.uk