James Furness

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Research Summary:

Density functional theory (DFT) has become the foremost computational method across materials science and chemistry, primarily due to its useful compromise of accuracy and efficiency. Despite this success, much work remains to be done in developing the next generation of DFT methods that extend the technique to ever more challenging and sensitive situations[11]. The past decade has seen much attention focussed on improving accuracy methods, to the extent that materials previously thought of as too complex for DFT have been successfully modelled [4], [7], [12], [13]. Often however, this advance in accuracy has been at the expense of computational efficiency, preventing the accuracy enabled new methods from being brought to bear in high-throughput studies for material or drug design. My research drive has been to address this disconnect by blending my molecular physics background with an expertise in numerical methods and computer programming to **design theoretical and computational tools that deliver cutting edge accuracy from minimal computer resources**[1], [5], [9]. This research goal is directed and informed by an overarching interest in improving the energy sustainability of humankind both by designing new tools for energy chemistry simulation[1], [9], [14], [15], and by applying said tools to analyse energy important processes[6], [7], [8], [10], [12], [13].

Education:

2016: Ph. D, Theoretical Chemistry, University of Nottingham
- Supervisor: Andrew M. Teale
- Thesis title: Extending Density Functional Theory to Molecules in Magnetic Fields

2013: M.Sci, Chemistry, University of Nottingham (1st class)

Professional Appointments:

2017 – present: Postdoc (Supervisor: Jianwei Sun), Dept. of Physics & Engineering Physics, **Tulane University**
2016 – 2017: Postdoc (Supervisor: Jianwei Sun), Physics Dept., **The University of Texas at El Paso**

Awards:

2020: Tulane University Supporting Impactful Publications Program ($1,750).
2017-2020: Tulane University Office of Postgraduate and Postdoctoral Studies Travel Award ($500), each year 2017-2020.
2017: The USA Department of Energy, Energy Frontier Research Center (EFRC) 'Sound ∩ Science Podcast Contest' outreach event – Main author of the Center for Complex Materials from First Principles (CCM) entry. Won "Best Science Music Composition".
2016: Dan Eley Prize – Awarded for "outstanding academic achievement and contribution to the activities of the physical chemistry section, school of chemistry and University of Nottingham".
2013: Kings Memorial Medal - Awarded for "outstanding project work in the final year of the Chemistry MSci degree".

Professional Activities:

Reviewer: The Journal of Physical Chemistry Letters, Physical Review B, Journal of Chemical Physics, MDPI: Materials, MDPI: Crystals, MDPI: Molecules, MDPI: Computation.

Member: American Physical Society (APS), American Chemical Society (ACS)

Editor: Editorial board for *Frontiers in Energy Research* newsletter (http://www.energyfrontier.us/newsletter) from the Office of Basic Energy Sciences at U.S. Department of Energy Office of Science.

Developer: Scientific programming expertise in Python, C++, and Fortran.
Contributions to Tubomole, VASP, XCFun, and the QUEST program codes.
In-development fork of pyscf implementing support for fractional nuclear charges.
Lead developer of efficient python atomic orbital code for rapid method development and testing.
Authored small open-source scientific tools.
Attended "New Horizons in Scientific Software: from Legacy Codes to Modular Environments" conference.
Installed, maintained, and administrated Tulane MaTComp group high performance compute server.
Simple website design and maintenance of personal and research group sites.

Grants:

2020: National Science Foundation career grant, under consideration. *Visualisation, interpretation, and modelling of exchange-correlation hole for density functional theory* ($500,000 significant contribution)

2018: Department of Energy, 09/01/2018-08/31/2021, $450,060, *Development of a local hybrid density functional to treat the self-interaction error and the nonlocal many-electron interaction* (significant contribution)

2018: American Chemical Society Petroleum Research Fund, 09/01/2018-08/31/2020, $110,000, *Understanding the asymptotic dependence of van der Waals density functionals for heterogeneous catalysis* (minor contribution)

Teaching Experience:

2017- Department of Physics and Engineering Physics, Tulane University

- FA2020, Computational Materials Science and Engineering (25 graduate and undergraduate students), gave guest lecture and created 3 lab classes.
- SP2020, Quantum Mechanics II (15 graduate students), lectured 2 classes.
- Mentored 4 Ph.D students.
- Created and ran two summer research placements for high-school students.

2016-2017 Physics Department, The University of Texas at El Paso

- SP2017, Quantum Mechanics (~20 graduate students), lectured 4 classes.
- Mentored 2 Undergraduate students.

2013-2016 Chemistry Department, The University of Nottingham

- F13CLC, Chemistry and Molecular Physics Literature and Communication Skills (40 undergraduate students), group tutor.
- F13ALA-F13ALC, Advanced Laboratory Chemistry (all Junior year undergraduate chemistry students, ~40 per class group), postgraduate laboratory demonstrator.
- Bash programming workshop (~15 graduate students), lecturer.
- Mentored 5 masters students.

Publications (Google Scholar citations: 379, h-index: 10, August/2021)

[1] G David, T Irons, A Fouda, J W Furness, A Teale, Self-Consistent Field Methods for Excited States in Strong Magnetic Fields: A Comparison Between Energy- and Variance-based Approaches. **J. Chem. Theory Comput.** Accepted, (2021)

[2] J W Furness, R. Zhang, and J. Sun, A paradigm system for strong correlation and charge transfer competition. *arXiv:2103.03178* (2021).

[3] J W Furness, A Kaplan, J Ning, J P Perdew, J Sun, Accurate and Numerically Efficient r^2SCAN meta-Generalized Gradient Approximation. **J. Phys. Chem. Lett** 11, 244112 (2020)

[4] Y Zhang, J W Furness, R Zhang, Z Wang, A Zunger, J Sun, Symmetry-Breaking Polymorphous Descriptions for Complex Materials without Interelectronic U. **Phys. Rev. B** 102(4), 045112 (2020)

[5] J W Furness, N Sengupta, J Ning, A Ruzsinszky, J Sun, Examining the order-of-limits problem and lattice constant performance of the Tao—Mo Functional. **J. Chem. Phys.** 152(June), 244112 (2020)

[6] C Lane, Y Zhang, J W Furness, R S Markiewicz, B Barbiellini, J Sun, A Bansil, First-Principles Calculation of Spin and Orbital Contributions to Magnetically Ordered Moments in Sr_2IrO_4. **Phys. Rev. B** 101(15), 155110 (2020)

[7] Y Zhang, C Lane, J W Furness, B Barbiellini, J P Perdew, R S Markiewicz, A Bansil, J Sun, Competing stripe and magnetic phases in the cuprates from first principles. **Proc. Natl. Acad. Sci.** 117(1) (2019)

[8] J Ning, J W Furness, Y Zhang, A C Thenuwara, R C Remsing, M L Klein, D R Strongin, J Sun, Tuneable catalytic activity of cobalt-intercalated layered MnO_2 for water oxidation through confinement and local ordering. **Journal of Catalysis** 374, 143-149 (2019)

[9] J W Furness, J Sun, Enhancing the efficiency of density functionals with an improved iso-orbital indicator. **Physical Review B**, *99*(4), 041119 (2019)

[10] Y Zhang, J W Furness, B Xiao, J Sun, Subtlety of TiO_2 phase stability: Reliability of the density functional theory predictions and persistence of the self-interaction error. **J. Chem. Phys.**, *150*(1), 014105 (2019)

[11] J Sun, J W Furness, Y Zhang, Chapter 4: Density Functional Theory. **Dev. Phys. Theor. Chem.**, edited by S. M. Blinder and J. E. B. T.-M. P. in T. C. House (Elsevier, 2019), pp. 119–159 (2019)

[12] C Lane, J W Furness, I G Buda, Y Zhang, R S Markiewicz, B Barbiellini, J Sun, A Bansil, Antiferromagnetic ground state of La2CuO4: A parameter-free ab initio description. **Physical Review B**, *98*(12), 125140 (2018)

[13] J W Furness, Y Zhang, C Lane, I G Buda, B Barbiellini, R S Markiewicz, A Bansil, J Sun, An accurate first-principles treatment of doping-dependent electronic structure of high-temperature cuprate superconductors. **Nature Communications Physics**, 1 (11), 1–6 (2018)

[14] T J P Irons, J W Furness, M S Ryley, J Zemen, T Helgaker, A M Teale, Connections between variation principles at the interface of wave-function and density-functional theories. **J. Chem. Phys.** 147 (13), 134107 (2018)

[15] J W Furness, U Ekström, T Helgaker, A M Teale, Electron localisation function in current-density-functional theory, **Mol. Phys.** 2016, 8976 (2016)

[16] J W Furness, J Verbeke, E I Tellgren, S Stopkowicz, U Ekström, T Helgaker, A M Teale, Current Density Functional Theory Using Meta-Generalized Gradient Exchange-Correlation Functionals, **J. Chem. Theory Comput.** 11 (9), 4169–4181 (2015)

[17] E I Tellgren, A M Teale, J W Furness, K K Lange, U Ekström, T Helgaker, Non-perturbative calculation of molecular magnetic properties within current-density functional theory, **J. Chem. Phys.** 140 (3), 034101–034112 (2014)

Invited Talks:

- Session Chair, APS March Meeting (Online, 2021) – *DFT and Beyond.*
- FLO-SIC All hands meeting, University of Texas at El Paso (Online, 2020) – *Accurate and efficient functionals by restoring exact constraints to the regularised-SCAN functional*
- FLO-SIC All hands meeting, University of Texas at El Paso (El Paso, 2019) – *Enhancing the efficiency of density functionals with an improved iso-orbital indicator*.

- CCM SCAN Workshop, Temple University (Philadelphia, 2018) – *Developing local hybrid functionals.*
- CCM SCAN Workshop, Temple University (Philadelphia, 2017) – *First principles description of doping dependent structure in high temperature superconductors.*

Contributed Talks:

- APS March Meeting, Online (March, 2021) - *Accurate and numerically efficient r^{2}SCAN meta-generalized gradient approximation.*
- APS March Meeting, Online (March, 2020) - *Restoring Exact Constraints to the Regularised-SCAN Functional.*
- APS March Meeting, Boston (March, 2019) - *Enhancing the efficiency of density functionals with an improved iso-orbital indicator*.
- ACS National Meeting and Expo., New Orleans (March, 2018) - *Utilizing Advanced Kinetic Energy Density Based Ingredients for Novel Local Hybrid Mixing Functions*.
- APS March Meeting, Los Angeles (March, 2018) - *Utilizing Advanced Kinetic Energy Density Based Ingredients for Novel Local Hybrid Mixing Functions*.