

Dr James C. Womack MRSC

Employment

2015 – Present **Postdoctoral research fellow**
University of Southampton, with Prof C.-K. Skylaris

Education

2010–2015 **University of Bristol**
PhD by Research in theoretical / computational chemistry
Supervised by Prof F. R. Manby

2005–2010 **University of Bristol**
BSc in Chemistry (First Class Honours)

1997–2005 **Torquay Boys' Grammar School**
A levels: Chemistry (A), Biology (A), English Literature (A), General Studies (A)
AS levels: Geography (A); GCSEs: 9 A*s, 2 As

Research experience

2015–Present **Postdoctoral research on linear-scaling density-functional theory**
University of Southampton, with Prof C.-K. Skylaris

2010–2015 **PhD research on molecular integrals in electronic structure methods**
University of Bristol, with Prof F. R. Manby

2009–2010 **BSc research project in electronic structure theory**
University of Bristol, with Prof F. R. Manby

Publications

DL_MG: A Parallel Multigrid Poisson and Poisson-Boltzmann Solver for Electronic Structure Calculations in Vacuum and Solution

J. C. Womack, L. Anton, J. Dziedzic, P. J. Hasnip, M. I. J. Probert, and C.-K. Skylaris, *J. Chem. Theory Comput.* **14**, 1412 (2018); doi: 10.1021/acs.jctc.7b01274

Electronically Excited States in Solution via a Smooth Dielectric Model Combined with Equation-of-Motion Coupled Cluster Theory

J. C. Howard, J. C. Womack, J. Dziedzic, C.-K. Skylaris, B. P. Pritchard, and T. D. Crawford, *J. Chem. Theory Comput.* **13**, 5572 (2017); doi: 10.1021/acs.jctc.7b00833

Implementation and optimisation of advanced solvent modelling functionality in CASTEP and ONETEP

J. C. Womack, L. Anton, J. Dziedzic, P. J. Hasnip, M. I. J. Probert, and C.-K. Skylaris (ARCHER eCSE technical report, 2017); <http://www.archer.ac.uk/community/eCSE/eCSE07-06/eCSE07-06.php>

Use of the rVV10 Nonlocal Correlation Functional in the B97M-V Density Functional: Defining B97M-rV and Related Functionals

N. Mardirossian, L. Ruiz Pestana, J. C. Womack, C.-K. Skylaris, T. Head-Gordon, and M. Head-Gordon, *J. Phys. Chem. Lett.* **8**, 35 (2017); doi: 10.1021/acs.jpcllett.6b02527

Self-consistent implementation of meta-GGA functionals for the ONETEP linear-scaling electronic structure package

J. C. Womack, N. Mardirossian, M. Head-Gordon, and C.-K. Skylaris, *J. Chem. Phys.* **145**, 204114 (2016); doi: 10.1063/1.4967960

Evaluating Many-Electron Molecular Integrals for Quantum Chemistry

J. C. Womack, PhD thesis, University of Bristol, Bristol, 2015; doi: 10.13140/RG.2.1.2485.3843

Density fitting for three-electron integrals in explicitly correlated electronic structure theory

J. C. Womack and F. R. Manby, *J. Chem. Phys.*, **140**, 044118 (2014); doi: 10.1063/1.4863136

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Prizes and recognition

2015	Coulson Prize for talk at RSC TCG Graduate Student Meeting, Manchester.
2013	Poster prize at 7th Molecular Quantum Mechanics Conference, Lugano.
2011–2013	Society of the Chemical Industry Scholarship, one of three awarded in 2011.
2007–2008	Thomas Malkin Prize, for academic performance in second year of degree. Shell Library Project Prize, for second year library project. RSC Local Section Prize, for achievement in practical work.
2006–2010	AstraZeneca Chemistry Bursary, for academic performance in first year of degree.