Abstract Submitted
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**State-of-the-art molecular applications of full configuration interaction quantum Monte Carlo** ROBERT E. THOMAS, CATHERINE OVERY, JAMES J. SHEPHERD, University of Cambridge, The University Chemical Laboratory, United Kingdom, GEORGE H. BOOTH, Department of Chemistry, Frick Laboratory, Princeton University, USA, ALI ALAVI, University of Cambridge, The University Chemical Laboratory, United Kingdom — Full configuration interaction quantum Monte Carlo (FCIQMC)[1] and its initiator adaptation (*i*-FCIQMC)[2] provide, in principle, exact (FCI) energies *via* a population dynamics algorithm of an ensemble of discrete, signed walkers in Slater-determinant space. We demonstrate that a novel choice of reference state has the potential to widen the scope of this already versatile method, and corroborate the finding that an extension of the algorithm to allow non-integer walkers can yield significantly reduced stochastic error without a commensurate increase in computational cost[3]. New applications of FCIQMC to transition-metal systems of general and biological interest are presented, many of which have, to date, posed serious challenges for traditional quantum chemical methods[45]. [1] G. H. Booth, A. J. W. Thom, and A. Alavi, J. Chem. Phys., 131, 054106 (2009) [2] D. M. Cleland, G. H. Booth, and A. Alavi, J. Chem. Phys., 132, 041103 (2010) [3] F. R. Petruzielo, A. A. Holmes, H. J. Changlani, M. P. Nightingale and C. J. Umrigar, arXiv:1207.6138 [4] N. B. Balabanov and K. A. Peterson, J. Chem. Phys., 125, 074110 (2006) [5] C. J. Cramer, M. Wloch, P. Piecuch, C. Puzzarini and L. Gagliardi, J. Phys. Chem. A, 110, 1991 (2006)

Robert E. Thomas
University of Cambridge, The University Chemical Laboratory,
United Kingdom

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