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**Linear-scaling and projector self-consistent DFT+U for electronic correlations in large systems** DAVID D. O'REGAN, MIKE C. PAYNE, Cavendish Laboratory, University of Cambridge, ARASH A. MOSTOFI, The Thomas Young Centre, Imperial College London — ONETEP is an *ab initio* total-energy and force code for which the computational effort scales linearly with the number of atoms, recently shown to scale up to 32,000 atoms on 64 cores [1][2]. Conventional exchange-correlation functionals are often unable to describe the electronic structure of biomolecules and metal-oxide nanostructures correctly, tending to under-localise states associated with transition metal sites. We show that non-orthogonal, generalised Wannier functions provide an efficient basis of projectors with which to describe these localised states, thus to construct a Hubbard-model like correction, DFT+U [3], to treat correlations. We demonstrate DFT+U calculations that are self-consistent over the charge density, Wannier projectors and interaction parameters. The tensorial character of the occupancy matrices, accounting for Wannier projector non-orthogonality, is discussed and illuminated numerically. We present a parallelised,linear-scaling implementation of the DFT+U energies and forces in ONETEP, providing for accurate calculations on large organometallic compounds and nanostructures. [1] C.-K. Skylaris, et. al. *J.Chem.Phys.* **122** 084119 (2005). [2] N. D. M. Hine, et. al. *Comp.Phys.Comm.* **180** 1041 (2008). [3] M. Cococcioni, S. de Gironcoli, *Phys.Rev.B.* **71** 035105 (2005).

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