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Implicit solvent model for linear-scaling first-principles electronic structure calculations HATEM H. HELAL, MIKE PAYNE, Theory of Condensed Matter, Cavendish Laboratory, University of Cambridge, ARASH A. MOSTOFI, Departments of Physics and Materials, Imperial College London — Density functional theory (DFT) enables first-principles calculations that exhibit cubic scaling of the computational time required with respect to the number of atoms in the system. This presents an unavoidable difficulty when first-principles accuracy is needed for the study of large-scale biological systems. The ONETEP program reformulates DFT so that the required computational effort scales only linearly with system size, recently demonstrated for up to 32,000 atoms on 64 cores.[1] Further complicating DFT based studies of biomolecular systems is the need for an accurate representation of the electrostatic environment. Rather than introducing explicit solvent molecules into the system, which would be computationally prohibitive, we present our recent efforts to integrate an implicit solvent model[2] with ONETEP in order to study systems in solution consisting of many thousands of atoms. We report preliminary results of our methodology with a study of the DNA nucleosome core particle.

[1]N. D. M. Hine, P. D. Haynes, A. A. Mostofi, C.-K. Skylaris and M. C. Payne, submitted to *J. Chem. Phys.* (2008).
[2]D. A. Scherlis *et al.*, *J. Chem. Phys.* **124**, 074103 (2006).

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