

Abstract Submitted
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Dispersion interactions with linear scaling DFT: a study of planar molecules on charged polar surfaces LAMPROS ANDRINOPOULOS, NICHOLAS HINE, PETER HAYNES, ARASH MOSTOFI, Imperial College London — The placement of organic molecules such as CuPc (copper phthalocyanine) on wurtzite ZnO (zinc oxide) charged surfaces has been proposed as a way of creating photovoltaic solar cells¹; optimising their performance may be aided by computational simulation. Electronic structure calculations provide high accuracy at modest computational cost but two challenges are encountered for such layered systems. First, the system size is at or beyond the limit of traditional cubic-scaling Density Functional Theory (DFT). Second, traditional exchange-correlation functionals do not account for van der Waals (vdW) interactions, crucial for determining the structure of weakly bonded systems. We present an implementation of recently developed approaches² to include vdW in DFT within ONETEP³, a linear-scaling package for performing DFT calculations using a basis of localised functions. We have applied this methodology to simple planar organic molecules, such as benzene and pentacene, on ZnO surfaces.

¹G.D. Sharma *et al.*, *Solar Energy Materials & Solar Cells* **90**, 933 (2006)

²P.L. Silvestrelli, P.R.L. **100**, 102 (2008)

³C.-K. Skylaris, P.D. Haynes, A.A. Mostofi and M.C. Payne, *J.C.P.* **122**, 084119 (2005)

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