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Title: Linear-scaling density-functional theory: from fundamental principles to practical applications

Name: Haynes, Peter

Affiliation: Imperial College London

It is 20 years since Yang proposed the first "divide-and-conquer" linear-scaling method [1]. Since then a lot of effort has been invested in the development of O(N) methods for density-functional theory (DFT), but relatively little seems to have resulted in terms of practical applications. In this talk I will suggest why this is the case and how it may be addressed. First, I will briefly outline the linear-scaling DFT scheme implemented in the ONETEP code [2], focusing on the in situ optimization of local orbitals that enables plane-wave accuracy to be achieved. I will suggest that the resulting "non-orthogonal generalized Wannier functions" may be used in a manner similar to maximally localized Wannier functions e.g. to interpolate band structure and to calculate changes in bulk polarization. Second, I will present results of simulations of polar semiconductor nanorods that are amenable to O(N) methods and demonstrate the sorts of questions and systems that can be studied successfully [3]. Finally I will present very recent work on the optimization of an additional set of local orbitals for unoccupied states that allow the calculation of optical absorption spectra and open up the way for future developments. [1] Phys. Rev. Lett. 66, 1438 (1991) [2] www.onetep.org [3] Phys. Rev. B 83, 241402 (2011)