Abstract Submitted
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Towards the calculation of experimental spectra using linear-scaling density-functional theory LAURA RATCLIFF, PETER HAYNES, Imperial College London — The theoretical calculation of spectra is highly useful both in understanding experimental results and making predictions about new materials. This work will combine the power of spectroscopy with the ability of linear-scaling density-functional theory (DFT) to study much larger systems than previously possible. A necessary first step involves finding a method to calculate conduction states and implementing it in ONETEP, a linear-scaling DFT code, which is currently limited to the calculation of valence states. These can then be used to calculate spectra using perturbation theory. A "toy model" has been created with a one-dimensional Kronig-Penney potential and a localised basis set of B-splines, which solves the generalized Schrödinger equation using a preconditioned conjugate gradient energy minimisation scheme, analogous to that of ONETEP. This program has been used to test the possible methods for calculating excited states before implementing in ONETEP.

[1] C.-K. Skylaris, P. D. Haynes, A. A. Mostofi, and M. C. Payne, J. Chem. Phys. **122**, 084119 (2005).

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