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**A linear-scaling implementation of time-dependent density-functional theory (TDDFT) in the linear-response formalism** TIM ZUEHLSDORFF, Imperial College London, NICHOLAS HINE, University of Cambridge, JAMES SPENCER, NICHOLAS HARRISON, JASON RILEY, PETER HAYNES, Imperial College London — In recent years, linear-scaling approaches to density functional theories have been successfully used to predict ground state properties of nanostructures and large biological systems. While these methods are now well established, the linear-scaling computation of excited state properties via time-dependent density-functional theory (TDDFT) remains challenging. In this talk, we will present a fully linear-scaling implementation of TDDFT in the linear-response formalism that we developed recently (J. Chem. Phys. 139, 064104) and that is particularly suitable for calculating the low energy absorption spectra of systems containing thousands of atoms. The method avoids any reference to individual Kohn-Sham states. Instead, the occupied and unoccupied subspaces are represented by two effective density matrices that are expanded in terms of two independent sets of in-situ optimized localized orbitals. The double basis set approach avoids known problems of representing the unoccupied space with localized orbitals optimized for the unoccupied space, while the in-situ optimization procedure allows for efficient calculations using a minimal number of basis functions. The linear-scaling properties of the method will be demonstrated on a number of nanostructures.

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