

CONDENSED MATTER PHYSICS SEMINAR

Thursday 6 November at 14:30

Simpkins Lee Seminar Room, Department of Physics

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Accurate Solid-State Band Gaps and Optical Absorption Spectra from Density Functional Theory

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Bandgaps and absorption spectra in the solid state are among the most important properties for determining the usefulness of materials in a wide range of areas, from photovoltaics to quantum materials. Ideally, we would like to deduce these properties from first principles calculations. However, the workhorse of such calculations, namely density functional theory (DFT), has traditionally struggled - even qualitatively - in the description of electron and optical excitations. Specifically, the bandgap of semiconductors and insulators has been thought to be outside the reach of DFT even in principle, and the associated optical absorption spectrum outside the reach of time-dependent DFT with standard approximate functionals. Charge transfer excitations have also presented significant difficulties in both molecular and solid-state systems.

Here, a novel approach to overcoming these difficulties, involving Wannier-localization based optimal tuning of a screened range-separated hybrid functional, is presented. It is shown that quantitative accuracy for a wide range of systems, from molecules to 3d and 2d materials, is achieved without any empiricism. This opens the door to many DFT-based true predictions of electronic and optical properties, to high-throughput calculations, and to a systematic choice of the starting point for many-body perturbation theory calculations.