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Reshaping the research landscape for the description of excited states in solids: the tool set of the CP2K-Newton-X program package

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The plethora of photochemical processes that need to be unraveled when aiming for a comprehensive description of excited states in solids becomes apparent when considering the process of upconversion: Converting two low energy photons to a high energy one is of vital importance for both catalytical as well as bio-medical applications, holding the promise to enhance both sensing, phototherapy, and theranostics as well as photocatalysis under low solar irradiance. The challenge of overcoming the systematically too low quantum yields demands an atomistic understanding of the full range of relevant photochemical mechanisms, emphasizing the need for an advanced quantum-mechanical tool set for the description of excited states within time-dependent density functional theory implying periodic boundary conditions. This presentation summarizes first steps towards setting up such a versatile tool set within the CP2K-Newton-X interface [1, 2], with recent developments enabling to go from static absorption and emission spectroscopy to non-adiabatic trajectory surface hopping beyond the classical path approximation [3,4].

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