DFTB+ for excited states: an overview of the TD-DFTB implementations, its features, applications, and future challenges.

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Over the past few decades, a range of methods have been developed to study the excited state properties for quantum chemistry and physics. Among these methods, time-dependent density functional theory (TD-DFT) is widely used to compute the excited states of several type of materials namely, crystals, low-dimensional materials, surfaces, nanomaterials, macromolecules, polymers, and biological systems. However, the computational complexity of TD-DFT, which typically scales in the order of $O(N^4)$/$O(N^5)$, makes it difficult to use for large systems, unless HPC clusters are available, which is not always the case. In this context, density functional tight-binding (DFTB) and its time-dependent version (TD-DFTB) offer promising alternatives for studying the ground and excited states of many materials. Compared to (TD-)DFT, (TD-)DFTB is typically 2-3 orders of magnitude faster while providing similar accuracy. Since its most recent implementation paper in 2020, DFTB+ [1] has been widely used by several groups (more than 400 citations in crossref), evidencing the increasing interest in the method and its applications among the users community. In this talk I will focus on the current state of TD-DFTB implementations in the DFTB+ code, specifically the linear-response [2] and real-time [3] implementations. I will provide a brief comparison of both methods, including their limitations and applications. The long-range corrected (LC) exchange-correlation functional implementation [4] will also be addressed in the context of TD-DFTB. Additionally, I will discuss the latest features that have been implemented in the code and the future challenges related to both approaches to tackle new phenomena and materials.

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