

Abstract Submitted  
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**Real-Time Subsystem TD-DFT and its Ehrenfest Dynamics: Applications to solvation and exciton transfer**<sup>1</sup> MICHELE PAVANELLO, Rutgers Univ - Newark — The subsystem formulation of DFT known as Frozen Density Embedding (FDE) provides a divide-and-conquer approach to Kohn–Sham DFT for a collection of weakly bound subsystems. We present theory and computer code development of the time-dependent extension of FDE. The code is now part of the Quantum–ESPRESSO suite of softwares. We also present the associated Ehrenfest dynamics, in which nuclei and electrons of selected subsystems are propagated simultaneously. Application of the code to exciton transfer phenomena as well as to solvatochromic shifts are discussed.

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