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New TDDFT Algorithms, Protocols and Analysis Tools for the Study of Optical Properties and Plasmons of Large Metal Clusters

A recent algorithm to solve the TDDFT equations in the space of the density fitting auxiliary basis set has been developed and implemented in ADF/AMS [1]. The TDDFT equations are recast to a non-homogeneous linear system, whose size is much smaller than in Casida formulation, allowing to calculate a wide portion of the absorption spectrum for large systems. The method extracts the spectrum from the imaginary part of the polarizability at any given photon energy, avoiding the bottleneck of Davidson diagonalization. The new algorithm also benefits from a recent very efficient extension to hybrid functionals [2,3] and is supported by many analysis tools. Recent applications to ligand protected [4], chiral metal clusters [5,6] and plasmonic systems [7] will show the potentiality of the method.

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