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Ab-initio Charge and Spin Dynamics in Solids using TDDFT[1]

PETER ELLIOTT, K KRIEGER, S SHARMA, J.K DEWHURST, E.K.U GROSS, Max Planck Institute for Microstructure Physics — With the advent of ultrafast and high intensity laser pulses, we can probe many new and interesting phenomena. Due to the time-scale of such situations, fully quantum mechanical approaches for the electron dynamics are required. Time-dependent density functional theory (TDDFT) is the natural choice for this problem, as it balances accuracy and efficiency. Here we report on the implementation of real time TDDFT for periodic systems including non-collinear magnetization, in the ELK electronic structure code[1]. This allows us to study situations beyond the usual linear-response, for example ultrafast demagnetization[2] or laser-induced dielectric breakdown. Additionally, we are developing and testing new methods related to time-dependent problems, such as an exchange-correlation magnetic field which is locally non-collinear[3], a time-dependent polarization field, and coupling to Maxwell's equations. [1] elk.sourceforge.org [2] Ab-initio Ultrafast Demagnetization in Solids, K. Krieger, P. Elliott, S. Sharma, J.K. Dewhurst, E.K.U. Gross, in prep (2013). [3] Transverse spin-gradient functional for noncollinear spin-density-functional theory, F.G. Eich and E.K.U. Gross, Phys. Rev. Lett. 111, 156401 (2013).

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