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Abstract for an Invited Paper for the MAR16 Meeting of the American Physical Society

Extensions of time density functional theory to QED: QED-Chemistry

ANGEL RUBIO, Max Planck fro the Structure and Dynamics of Matter

n this talk we will review the recent advances within density-functional and many-body based schemes to describe spectroscopic properties of complex systems with special emphasis to modelling time and spatially resolved electron spectroscopies We will discuss the theoretical approaches developed in the group for the characterisation of matter out of equilibrium, the control material processes at the electronic level and tailor material properties, and master energy and information on the nanoscale to propose new devices with capabilities. We will focus on examples linked to the efficient conversion of light into electricity or chemical fuels ("artificial photosynthesis") and the design on new nanostructured based optoelectronic devices based on inorganic nanotubes, among others. The goal is to provide a detailed, efficient, and at the same time accurate microscopic approach for the ab-initio description and control of the dynamics of decoherence and dissipation in quantum many-body systems. With the help of quantum optimal control (QOC) theory and the mastery over spectroscopy we could direct the movement of electrons, selectively trigger chemical reactions and processes, and create new materials