UNIVERSITÄT DUISBURG ESSEN

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Ultrafast charge and spin dynamics in functional materials: insights from beyond DFT methods

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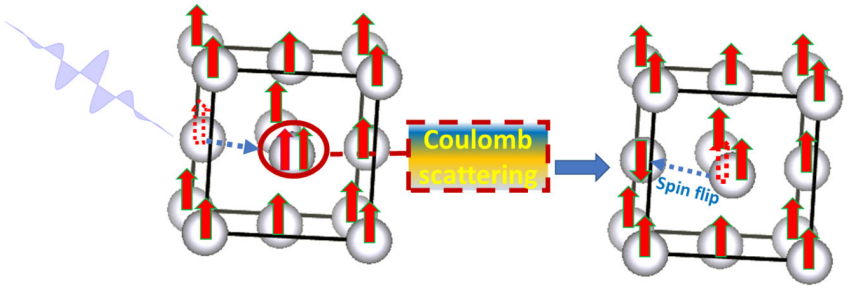

Experimental observations of the ultrafast (> 50 fs) demagnetization of Ni made two decades back had defied theoretical explanations for several reasons: its spin-flipping time is much less than that resulting from spin orbit and electron-lattice interactions and standard theoretical methods may not capture the role of electron correlations. Recent advances in theoretical techniques which combine time-dependent spin density-functional theory (TDDFT) and dynamical mean-field theory (DMFT) have enabled the inclusion of electron correlations, as well as the time dependence of electron-electron interaction. In this talk, I will present results of application of the TDDFT+DMFT to Ni which show that indeed the demagnetization occurs at the femtosecond scale [1], in good agreement with experimental observations, and that this ultrafast demagnetization results mainly from spin-flip transitions from occupied to unoccupied orbitals implying a dynamical reduction of exchange splitting. These conclusions are found to be valid for a wide range of laser pulse amplitudes. Similarly, I will relate the insulator to metal transition in VO_2 to the time-dependence of the excited charge density [2]. Here the time-dependence of the chemical potential of the excited electron and hole subsystems shows that even for such short times the dynamics of the system is significantly affected by memory effects—the time-resolved electron–electron interactions. The above results pave the way for obtaining a microscopic understanding of the ultrafast dynamics of strongly-correlated materials.

[1] S. R. Acharya *et al.*, Phys. Rev. Lett. **125**, 017202 (2020).

[2] J. M. Galicia-Hernandez, J. Phys.: Condens. Matter **32**, 20LT01(2020).