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"Light-induced changes of couplings in materials: Enhanced electron-phonon coupling, reduced Hubbard U"

I will discuss recent progress in the theoretical understanding of the modification of materials properties by ultrafast laser pulses:
(1) Enhancement of electron-phonon coupling in bilayer graphene by resonant phonon pumping [1, 2].
(2) Ultrafast modification of dynamical Hubbard U in NiO from first principles [3].
In (1) I will show combined theoretical and experimental evidence for enhanced coupling from time-resolved photoemission and THz spectroscopies [1] and a possible theoretical explanation invoking nonlinear electron-phonon coupling [2]. The latter could pave the way for „quantum nonlinear phononics“. In (2) I will show theoretical work on laser-driven NiO within a time-dependent density functional theory (LDA+U) calculation. Here the laser excitation is shown to reduce the self-consistent Hubbard U in a charge transfer insulator. As an example we compute the resulting high-harmonic generation (HHG) and show that the modified U changes the HHG significantly compared to a calculation with frozen U. Possible future avenues and open problems will be discussed.

[1] E. Pomarico et al., Phys. Rev. B 95, 024304 (2017).
[2] M. A. Sentef, Phys. Rev. B 95, 205111 (2017).
[3] N. Tancogne-Dejean, M. A. Sentef, and A. Rubio, in preparation