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Optimizing laser pulses for controlled excitation of materials and molecules[1] ROLAND ALLEN, Texas A&M University — This talk extends the ideas of recent papers, including [1] Zhou et al., Phys. Rev. B 82, 075433 (2010); [2] Lin et al., J. Phys. Cond. Mat. 21, 485503 (2009); and [3] Allen, Phys. Rev. B 78, 064305 (2008). There are three basic points: (1) A combination of analytical models and density-functional-based simulations provides guidance for tailoring laser pulses to achieve optimum vibrational and electronic excitation. In [1] it was found that the maximum relative response of a specific vibrational mode with period T is achieved when the FWHM duration of a pulse is equal to 0.42 T, and later work by Jiang et al. provided a similar criterion for the duration and delay times in a series of pulses. (2) It is possible for microscopic (density-functional-based) simulations to provide input for larger-scale simulations, in the form of stresses etc. (as demonstrated in [2]) and excitation-dependent interatomic potentials. (3) It is possible to extend current techniques for simulations of the coupled dynamics of electrons, nuclei, and the radiation field in highly-excited materials, using for example nonequilbrium Green's functions.

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