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Non-adiabatic simulations of terahertz manipulation of electronic excitations of Jahn-Teller active transition metal complexes using non-linear phononics.[1] OSCAR GRANAS, Uppsala University — Recent progress in laser technology has enabled the control of particular infra red (IR) active vibrational modes in molecules and solids. For cases when the activated IR modes couple to Raman active modes, it is possible to pump Jahn-Teller (JT) modes in compounds that where the electronic configuration is not JT active. Exciting the JT vibrational mode of transition metal complexes that are electronically JT active in the excited state, e.g. $[Ni(H_2O)_6]^{2+}$, facilitates a route to manipulate particular electronic excitations by enforcing a vibrational structure of the excited potential energy surface. We employ time-dependent density-functional theory in conjunction with Ehrenfest dynamics to simulate the process, describing ionic motion, external electromagnetic fields and evolution of the electronic wave-functions on the pico-second time-scale with realistic laser fluence.[2] The result sheds light on how coherent terahertz light influences the electronic degrees of freedom in open *d*-shell transition metal complexes.

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[2]G. Kolesov *et al.* J. Chem. Theory Comput.,12, pp 466-476; doi: 10.1021/acs.jctc.5b00969 (2016)

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