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Electron-phonon coupling effect on the vibrational relaxation of CO on Pd(111)

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The internal stretch mode of polar molecules adsorbed on metallic surfaces has emerged as an exceptional test-bed in which to probe many-body theories in current state-of-the-art time-revolved spectroscopy experiments. Here we study non-adiabatic effects on the internal stretch mode of CO adsorbed on the Pd(111) surface by means of first principles calculations [1, 2]. The theoretical
treatment that we employ, including electron-hole pair excitations and electron-mediated coupling between the vibrational modes [3, 4], allows us to study the internal stretch mode under thermal and non-thermal conditions. The latter permits to simulate the conditions that a femtosecond infrared pump pulse generates on the system and to predict the transient red-shift and change in the linewidth
that are induced. The laser-induced non-thermal electron and phonon distributions are described, respectively, by Fermi-Dirac and Bose-Einstein distributions defined by time-dependent electronic Te(t) and lattice Tl(t) temperatures are calculated with a two temperature model (TTM).

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