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Giant nonadiabatic effects in layer metals: Raman spectra of intercalated graphite and doped graphene explained. A. MARCO SAITTA, MICHELE LAZZERI, MATTEO CALANDRA, FRANCESCO MAURI, IMPMC, Paris, France — The occurrence of nonadiabatic effects in the vibrational properties of metals has been predicted since the 1960s [1], but hardly confirmed experimentally. We report the first fully ab initio calculations of nonadiabatic frequencies of a number of conventional (hcp Ti and Mg), layered metals (MgB2, CaC6, other intercalated graphites) [2] and doped graphene [3]. Nonadiabatic effects can be spectacularly large (up to 30% of the phonon frequencies), but they can only be experimentally observed in the Raman spectra of layered compounds. In layered metals nonadiabatic effects are crucial to explaining the observed Raman shifts and linewidths. Moreover, we show that those quantities can be used to extract the electron momentum-relaxation time. [1] S. Engelsberg and J.R. Schrieffer, Phys. Rev. 131, 993 (1962). [2] A.M. Saitta et al., Phys. Rev. Lett. 100, 226401 (2008). [3] M. Lazzeri and F. Mauri, Phys. Rev. Lett. 97 , 266407 (2006).

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