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Strong electron-phonon interaction in an FeSe monolayer¹ SINISA COH, MARVIN L. COHEN, STEVEN G. LOUIE, UC Berkeley, Lawrence Berkeley National Laboratory — We show that the electron-phonon coupling in an FeSe monolayer on a SrTiO₃ substrate is significantly larger than in earlier theoretical estimates. The role of the SrTiO₃ substrate is two-fold. First, the interaction of the FeSe and TiO₂ terminated face of SrTiO₃ prevents the FeSe monolayer from undergoing a shearing-type (orthorhombic) structural phase transition. Second, the substrate allows an anti-ferromagnetic ground state of FeSe which opens certain electron-phonon coupling channels within the monolayer that are prevented by symmetry in the non-magnetic phase. The spectral function for the electron-phonon coupling ($\alpha^2 F$) in our calculations agrees well with inelastic tunneling data.

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Sinisa Coh UC Berkeley and Lawrence Berkeley Natl Lab

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