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First-Principles Study of Superconductivity in Ultra- thin Pb Films JESSE NOFFSINGER, MARVIN L. COHEN, Deptartment of Physics, University of California, Berkeley; Materials Science Division, Lawrence Berkeley National Laboratory — Recently, superconductivity in ultrathin layered Pb has been confirmed in samples with as few as two atomic layers [S. Qin, J. Kim, Q. Niu, and C.-K. Shih, Science 2009]. Interestingly, the prototypical strong-coupling superconductor exhibits different T_c's for differing surface reconstructions in samples with only two monolayers. Additionally, T_c is seen to oscillate as the number of atomic layers is increased. Using first principles techniques based on Wannier functions, we analyze the electronic structure, lattice dynamics and electron-phonon coupling for varying thicknesses and surface reconstructions of layered Pb. We discuss results as they relate to superconductivity in the bulk, for which accurate calculations of superconducting properties can be compared to experiment [W. L. McMillan and J.M. Rowell, PRL 1965]. This work was supported by National Science Foundation Grant No. DMR07-05941, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the Lawrencium computational cluster resource provided by the IT Division at the Lawrence Berkeley National Laboratory (Supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231)

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