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Phonon-driven superconductivity in the vicinity of ferroelectric and charge density wave ordering in La(O,F)BiX_2 (X=S, Se, O) TANER YILDIRIM, National Institute of Standards and Technology — Examples of layered superconductors include cuprates, MgB_2, CaC_6, and recent iron-pnictides. Recently a new family of layered materials containing BiS_2 planes, was discovered to be superconducting at temperatures up to 10 K. In order to reveal the mechanism of superconductivity, here we present results from first-principles calculations with many surprising findings for La(O,F) Bi X_2 for X=S, Se, and O. The parent compound $LaOBiS_2$ possesses anharmonic ferroelectric soft phonons at the zone center with a rather large polarization of P $\approx$ 10 μC/cm^2. Upon electron doping, new unstable phonon branches appear along the entire line Q=(q,q,0), causing Bi/S atoms to order in a one-dimensional charge density wave (CDW). We find that BiS_2 is a strong electron-phonon coupled superconductor in the vicinity of competing ferroelectric and CDW phases. We discuss similar results for X=Se and hypothetical compound X=0. These results will be compared with another interesting system, namely $Ba_{1-x}K_xBiO_3$, which exhibits several phases, including CDW, an incommensurate pseudo ferroelectric, and superconductivity at 31 K. Our results suggest new directions to tune the balance between these phases and increase T_c in this new class of materials.

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