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Ferroelectric Soft Phonons, Charge Density Wave Instability, and Strong Electron-Phonon Coupling in BiS_2-Layered Superconductors TANER YILDIRIM, NIST, Gaithersburg, MD and UPENN, Philadelphia, PA — Very recently a new family of layered materials, containing BiS_2 planes was discovered to be superconducting at temperatures up to T_c=10 K, raising questions about the mechanism of superconductivity in these systems. Here, we present state-of-the-art first principles calculations that directly address this question and reveal several surprising findings [1]. The parent compound $LaOBiS_2$ possesses anharmonic ferroelectric soft phonons at the zone center with a rather large polarization of $\approx 10\mu C/cm^2$, which is comparable to the well-known ferroelectric $BiFeO_3$. 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. Our results suggest new directions to tune the balance between these phases and increase T_c in this new class of materials.

[1] T. Yildirim, arXiv:1210.2418 (2012).

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