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Pressure-induced insulator-metal and structural transitions of $BaBiO_3$ from first principles LDA+U DAVIDE CERESOLI, SISSA, Trieste, ERIO TOSATTI, SISSA and ICTP, Trieste — At zero pressure and temperature $BaBiO_3$ is an insulator with a structural dimerization, equivalent to a static valence disproportionation of the two Bi ions per cell from 4+ to 3+/5+. Under pressure one would expect an insulator-metal transition and the eventual disappearance of the dimerization. Moreover, the metallic phase should be superconducting, in analogy the metal doped $Ba_{1-x}K_xBiO_3$ compounds. To date, there are no accurate ab initio predictions under pressure, essentially because LDA or GGA fail to stabilize an insulating phase with the correct distortion and electronic gap. We carried out first principles LDA+U calculations by determining the effective Hubbard U self-consistently at every pressure, and found that the presence of U is mandatory for a correct description of the zero-pressure state. Upon increasing pressure, we found an insulator to metal transition at $\sim$ 20 GPa. By further increasing the pressure, we predict the appearance of a superconducting phase, characterized by quantum melting of the weakly dimerized CDW lattice. The dimerization tendency and superconductivity are expected to weaken only at much higher pressures, presently under investigation.

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