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Correlation effects in charge-density wave insulator $BaBiO_3$
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The negative-U nature of $BaBiO_3$ leads to a charge-ordered insulating state in which pentavalent Bi^{5+} coexists with trivalent Bi^{3+}. Despite the apparent absence of strong-correlation effects in $BaBiO_3$ standard density functional (DFT) theory yields a much too small band gap of 0.14 eV. By means of an hybrid-DFT approach combined with self-consistent GW including vertex corrections we investigate the electronic, vibrational and dielectric properties of $BaBiO_3$. We show that the inclusion of strong-correlation effects increases the band gap up to 1.2 eV, shifts the oxygen breathing modes upwards by ≈ 2 THz and reduces the dielectric constant by a factor of 3. The overall agreement with available experimental data is significantly improved.

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