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134: 213026k **First−principles study of structural, electronic, dynamical, and dielectric properties of zircon.** Rignanese, G.−M.; Gonze, X.; Pasquarello, Alfredo (Unite de Physico−Chimie et de Physique des Materiaux, Universite Catholique de Louvain, B−1348 Louvain−la−Neuve, Belg.). *Phys. Rev. B: Condens. Matter Mater. Phys.* **2001**, 63(10), 104305/1−104305/7 (Eng), American Physical Society. We investigate structural, electronic, dynamical, and dielec. properties of zircon ($ZrSiO_4$) within d.−functional theory. The at. structure is fully relaxed and the structural parameters are found to differ by less than 1.5[percent] from the exptl. data. The assocd. electronic band structure and d. of states are also presented. Using d.−functional perturbation theory, we obtain the phonon frequencies at the center of the Brillouin zone, the Born effective charge tensors, and the dielec. permittivity tensors. The calcd. phonon frequencies agree with the IR and Raman exptl. values (rms relative deviations of 2.5[percent]) when available, while the silent modes are predicted to range between 119.6 and 943.3 cm^{-1}. We compute the Born effective charge tensors, that are found to be quite anisotropic. The electronic and static dielec. permittivity are analyzed in detail. Their difference is mostly due to the lowest IR−active mode, whose eigenvector corresponds to a distortion of the SiO_4 tetrahedra with a displacement of Zr and O atoms in opposite directions.

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