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First principles investigations of structural, elastic, dielectric and piezoelectric properties of {Ba,Sr,Pb}TiO_3, {Ba,Sr,Pb}ZrO_3 and {Ba,Sr,Pb}{Zr,Ti}O_3 ceramics BERNA AKGENC, Kirklareli University Department of Physics, Faculty of Science, Kavakli, 39060, Kirklareli, Turkey, CETIN TASSEVEN, Department of Physics, Faculty of Science, Yildiz Technical University, Davutpasa Campus, Esenler, 34210, Istanbul, Turkey, TAHIR CAGIN, Department of Materials Science and Engineering, Texas A&M University, College Station, TX 77843-3003, USA — We use first-principle density-functional study of structural, anisotropic mechanical, dielectric and piezoelectric properties of {Ba,Sr,Pb}TiO_3, {Ba,Sr,Pb}ZrO_3 and {Ba,Sr,Pb}{Zr,Ti}O_3 alloys in cubic perovskite structures at zero temperature. Because there is significant interest in finding new piezoelectrics that do not contain toxic elements such as lead. In this study, we compare piezoelectric response of those alloys to synthesize outstanding piezoelectric materials. In perovskite structures, the spontaneous polarization is due to enormous values of Born effective charges computed by linear response within density functional perturbation theory, which are much larger than predicted nominal charge. We deeply investigated the effects of composition, order and site defects structure on piezoelectric constants.

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