Effect of pressure on the global and local properties of cubic perovskite crystals

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Abstract :

The influence of pressure on the structural, elastic, thermal and bonding properties of four perovskite-type oxides AMO_3 is studied from the point of view of the quantum theory of atoms in molecules. Ab initio investigations are performed by means of the full-potential linear augmented plane-wave method as implemented in the wien2k code. The integrated basin charges resulting from the topological analysis of electronic density provide a partition of the bulk modulus and compressibility into atomic contributions. Special attention is paid to the nonlinear behaviour of the local bonding properties.

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