Bonding nature of alkaline earth oxides and semicore electrons

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Pressure-induced B1-B2 transition pressure, the elastic stability, etc. of MgO are singular compared with other alkaline earth oxides. We have recently found that in alkaline earth oxides except MgO there are core electrons interacting to the oxygen 2s state (semicore state) using the electronic state calculating method based on the density functional theory and the local density approximation. In the present study calculations of the electronic structures, the lattice energies, and the elastic characteristics are performed to understand the origin of the differences between MgO and other alkaline earth oxides and to nvestigat the role of the semicore state of cations in alkaline earth oxides. All the calculations are based on the first-principles Full-Potential Linear Muffin-Tin-Orbital (FPLMTO) method. We find that by excluding the semicore-O2s interaction from the electronic structures, the properties of CaO, SrO and BaO approach those of MgO. This suggests that the differences between MgO and other alkaline earth oxides relate to the existence of particular semicore electron in Ca, Sr and Ba, rather than the particularity of Mg.