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Strain-induced ferroelectricity in simple rocksalt binary oxides ERIC BOUSQUET, NICOLA SPALDIN, University of California Santa Barbara (USA), PHILLIPE GHOSEZ, Liege University (Belgium) — Rock salt binary AO oxides form an important family of compounds which was intensively studied, both experimentally and theoretically. In comparison to multifunctional ferroelectric perovskite oxides, their practical applications remain however limited and the emergence of ferroelectricity and related functional properties in simple binary oxides seems so unlikely that it was never previously considered. Here, we first show from first-principles density functional calculations that ferroelectricity can be easily induced in simple alkaline earth binary oxides such as BaO using appropriate epitaxial strains. We point out that the functional properties (polarization, dielectric constant and piezoelectric response) of such strained binary oxides are comparable in magnitude to those of typical ferroelectric perovskite oxides, so making them of direct interest for applications. Going further, we also show the possibility to induce ferroelectricity in the ferromagnetic rock salt binary oxides EuO, and so suggesting a new route to achieve multiferroism at high temperature by combining ferroelectric and magnetic properties in very simple structures.

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