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Domain walls in a perovskite oxide with two primary structural order parameters: first-principles study of $BiFeO_3$ OSWALDO DIÉGUEZ, ICMAB-CSIC and Rutgers University, PABLO AGUADO-PUENTE, JAVIER JUNQUERA, Universidad de Cantabria, JORGE ÍÑIGUEZ, ICMAB-CSIC — We present a first-principles study of ferroelectric domain walls (FE-DWs) in multiferroic $BiFeO_3$ (BFO), a material in which the FE order parameter coexists with anti-ferrodistortive (AFD) modes involving rotations of the O_6 octahedra. We find that the energetics of the DWs are dominated by the capability of the domains to match their O_6 octahedra rotation patterns at the plane of the wall, so that the distortion of the oxygen groups is minimized. Our results thus indicate that, in essence, it is the discontinuity in the AFD order parameter, and not the change in the electric polarization, what decides which crystallographic planes are most likely to *host* BFO's FE-DWs. Such a result clearly suggests that the O_6 rotational patterns play a primary role in the FE phase of this compound, in contrast with the usual (implicit) assumption that they are subordinated to the FE order parameter. Interestingly, we find that the structure of BFO at the most stable DWs resembles the atomic arrangements that are characteristic of low-lying (meta)stable phases of the material. Our work thus contributes to shape a coherent picture of the structural variants that BFO can present and the way in which they are related.

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