Bloch-type domain walls in rhombohedral BaTiO$_3$ MARYAM TAHERINEJAD, DAVID VANDERBILT, Rutgers University, PAVEL MARTON, VILGELMINA STEPKOVA, JIRI HLINKA, Academy of Sciences of the Czech Republic — Ferroelectric domain walls (FDWs) are usually considered to be of Ising type, but there have been suggestions in recent years that Bloch-type FDWs, in which the polarization rotates in the plane of the FDW, are also possible. The mechanically compatible and electrically neutral FDWs in rhombohedral BaTiO$_3$ are of $71^\circ$, $109^\circ$, and $180^\circ$ type. We have investigated these FDWs based both on first-principles calculations and on a Ginzburg-Landau-Devonshire (GLD) model.$^1$ The results from both approaches confirm the Ising nature of the $71^\circ$ FDW and the Bloch nature of the $180^\circ$ FDW, and predict both Ising-type and Bloch-type FDWs are possible for the $109^\circ$ case. Considering the relatively small rhombohedral strain in BaTiO$_3$, the competition between the energies of Bloch and Ising FDWs can be discussed in terms of a picture in which a Bloch wall is regarded as being composed of a pair of smaller-angle Ising ones. A reduction by 40% in the parameters describing the gradient term in the GLD model brings it into better agreement with the first-principles results for detailed properties such as the energies and widths of the FDWs.