Supplemental Material for Structural and thermal transport properties of ferroelectric domain walls in GeTe from first principles

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CONVERGENCE STUDY FOR FERROELECTRIC DOMAIN WALLS WITH RESPECT TO THE DOMAIN SIZE

We have performed the convergence study for the structural properties of ferroelectric domain walls (DWs) in GeTe with respect to the domain size. To reduce the computational time needed for the study here we relax Te atoms only, keeping the lattice vectors and Ge atom positions fixed. The widths and energies of $(11\bar{1})$ domain walls are shown in Table **??**. We can see that the 64 atom supercell is sufficiently large for 39° and 141° DWs since it gives the similar values of domain wall widths and energies compared to larger cells. For 180° DWs the convergence is reached for the 80 atoms supercell.

39° DW	H-H DW width [Å]	T-T DW width [Å]	DW energy [mJ/m^2]
64 atoms	2.47	6.13	1198
96 atoms	2.47	6.11	1170
104 atoms	2.70	6.13	1205
141° DW	H-T DW width [Å]	T-H DW width [Å]	DW energy [mJ/m^2]
64 atoms	4.03	4.33	1070
96 atoms	4.15	4.49	1056
104 atoms	4.14	4.40	1075
180° DW	H-H DW width [Å]	T-T DW width [Å]	DW energy [mJ/m^2]
64 atoms	12.45	11.44	772
80 atoms	13.60	16.11	966
104 atoms	13.75	16.16	955

TABLE I. Domain wall (DW) widths and energies for different sizes of the simulation supercell relaxing only Te atom positions.

The same convergence study for the hexagonal domain walls is presented in Fig. **??**. Converging results for these domain walls was more challenging mostly due to the larger number of atoms in the hexagonal unit cell. Additionally, the bound charge at (111) domain walls is larger compared to $(11\bar{1})$ DWs. causing larger electrical field along the domain tahat

makesthe relaxation of these domain walls more challenging. We can see that the sufficient convergence was achieved for the 144 atoms supercells.

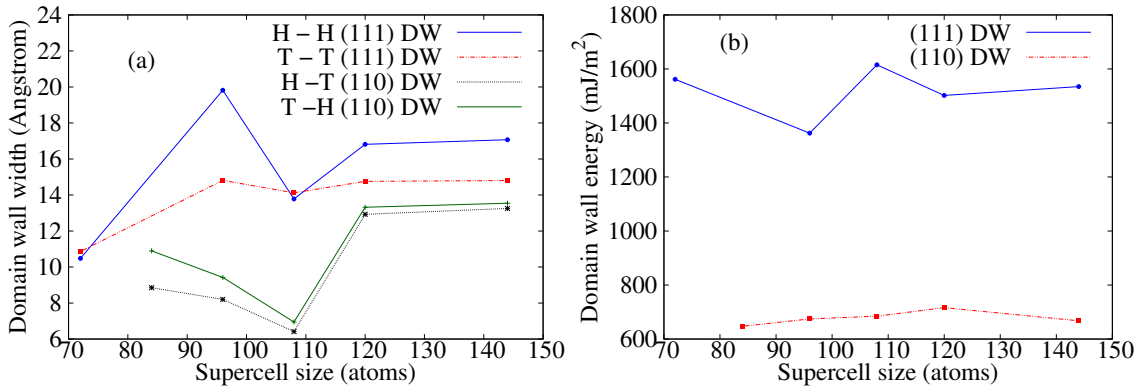

FIG. 1. (a) Domain wall width and (b) domain wall energy for (111) and $(1\bar{1}0)$ domain walls (DWs) as a function of the supercell size.