

## **Electronic supplementary information**

Atomistic prediction on the configuration- and temperature-dependent dielectric  
constant of Be<sub>0.25</sub>Mg<sub>0.75</sub>O superlattice as a high-κ dielectric layer

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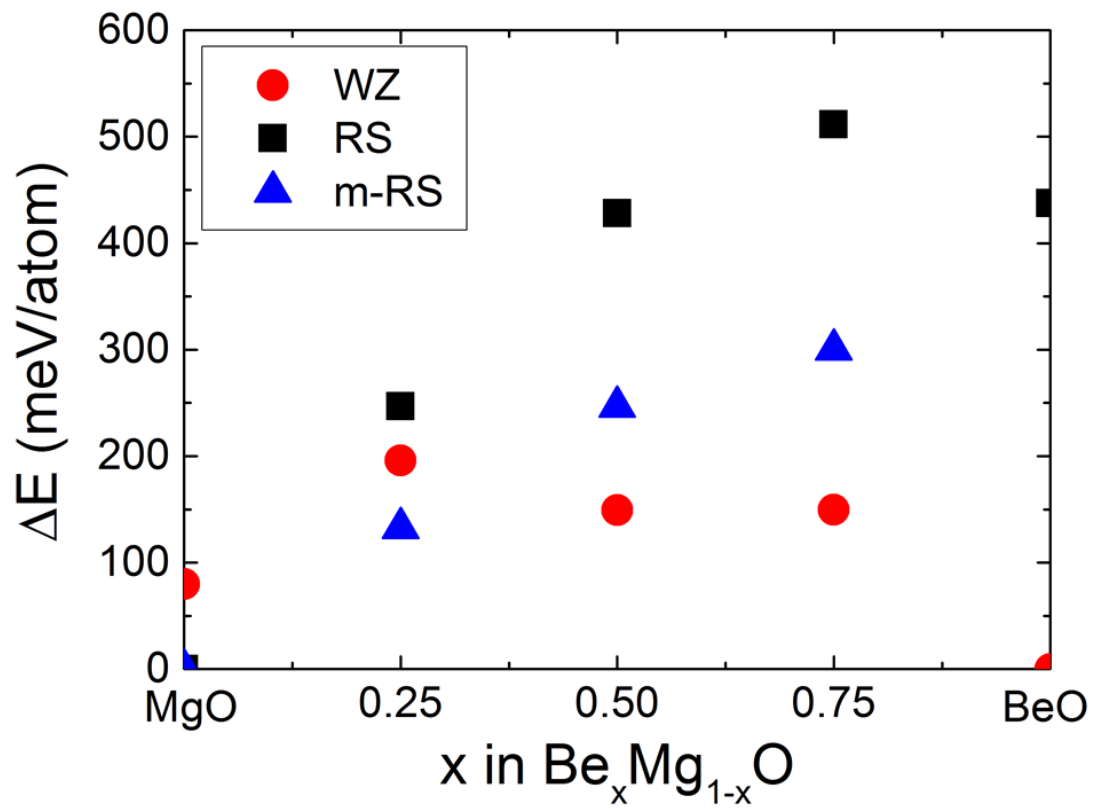


Figure S1.

Calculated  $\Delta E$  of WZ, RS, m-RS  $\text{Be}_x\text{Mg}_{1-x}\text{O}$  in 8-atom cell.

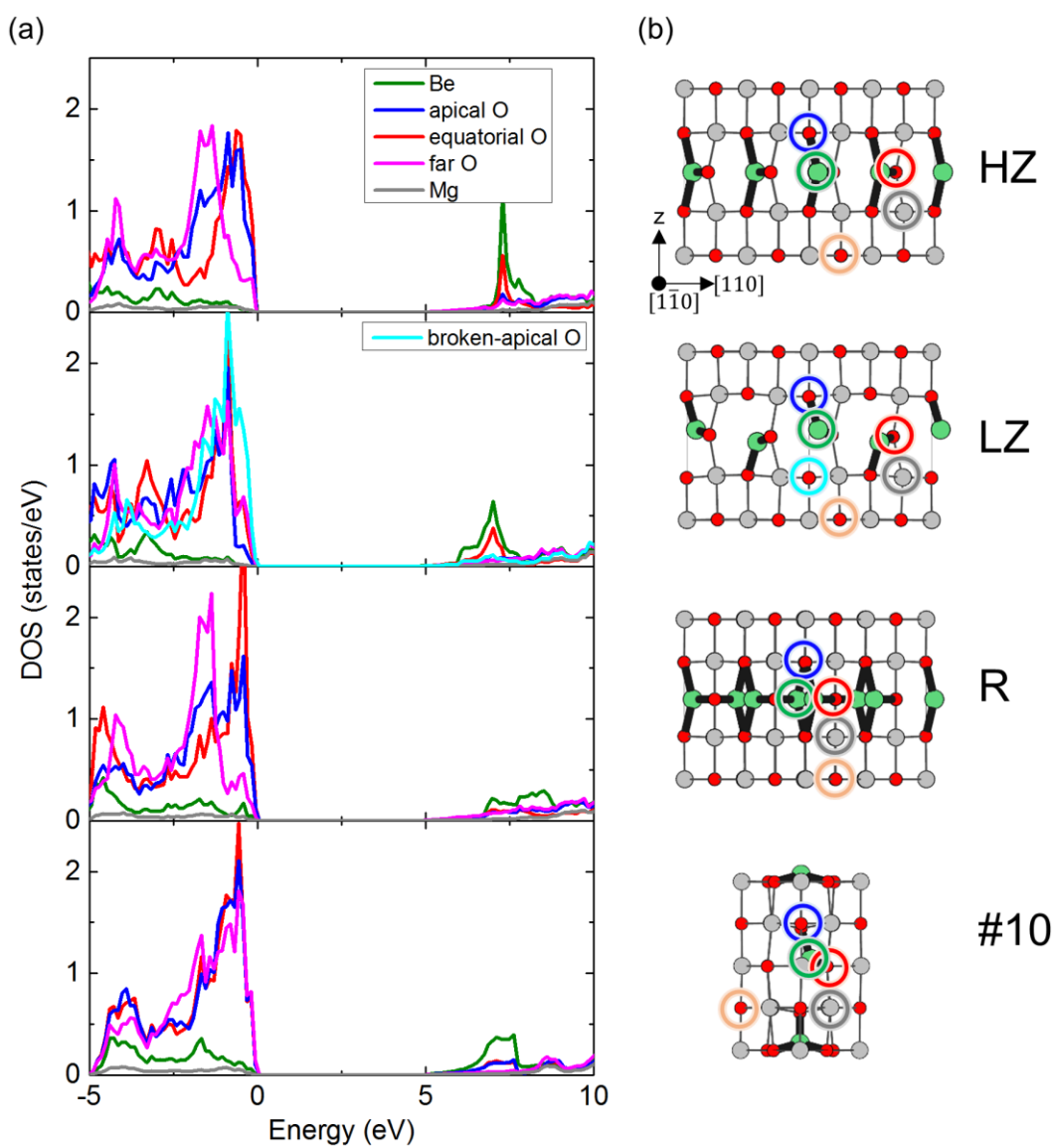


Figure S2.

(a) Partial density of states of *HZ*, *LZ*, *R*, and #10 and (b) corresponding atoms in each configuration marked by circles.

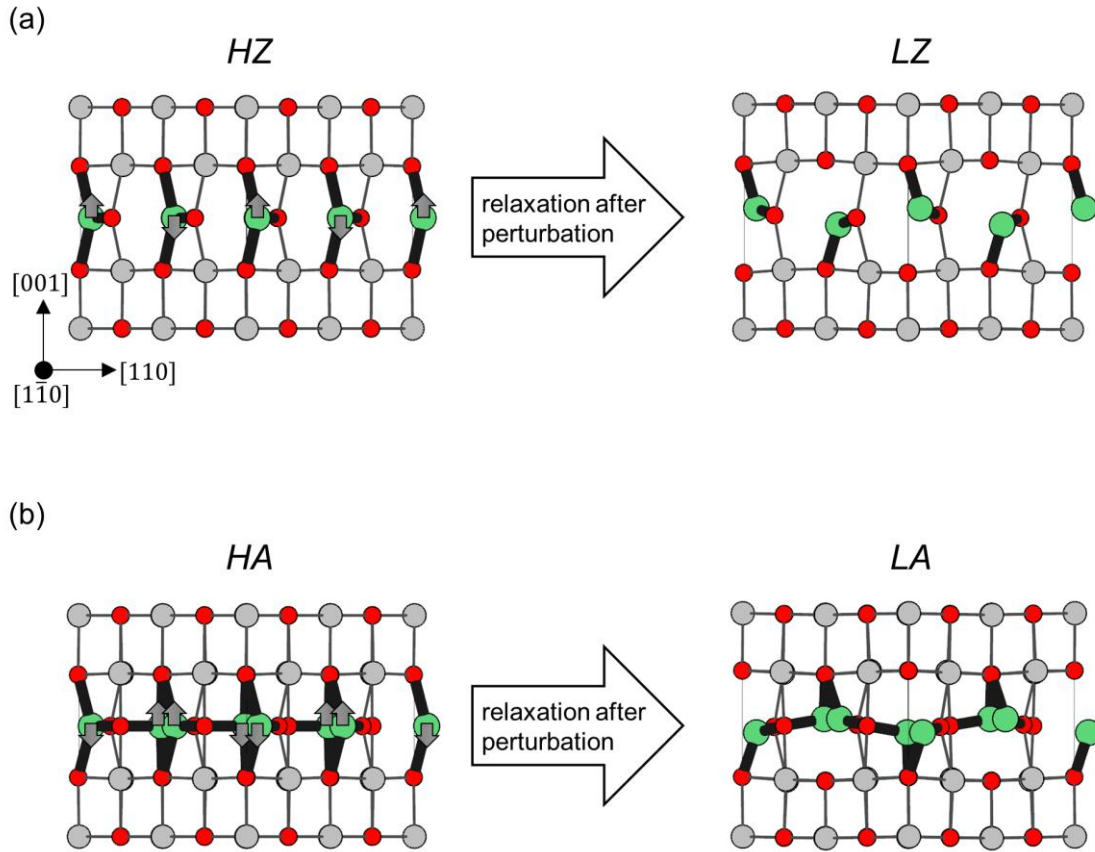


Figure S3.

Atomic positions of (a) *HZ* and *LZ* (b) *HA* and *LA*. The gray arrows indicate the atomic displacement induced by the phonon modes with the most negative eigenvalue at  $\Gamma$  of the high- $\kappa$ -type. When the atomic structure of the high- $\kappa$ -type is relaxed after a small perturbation along the atomic displacement by this phonon mode, configurations change from the high- $\kappa$ -type to the low- $\kappa$ -type.