Electronic Supplementary Material (ESI) for Nanoscale Horizons.

Supporting Information

Depolarization Induced III-V Triatomic Layers with Tristable Polarization States

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I. POLARIZATION OF III-V TRIATOMIC LAYERS

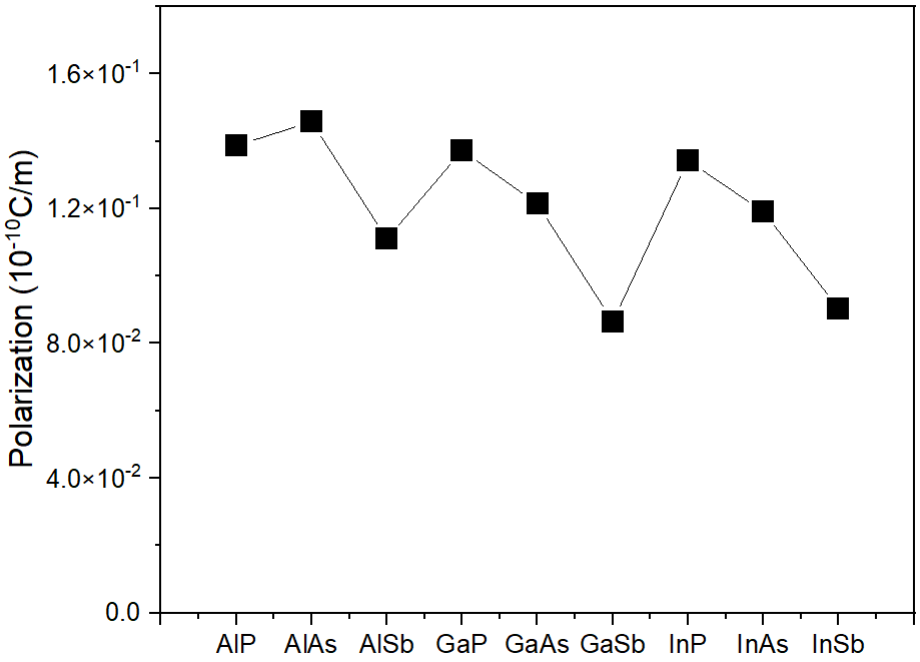

FIG. S1. Out-of-plane polarization of III-V triatomic layers.

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II. ANTIFERROELECTRIC ORDERING

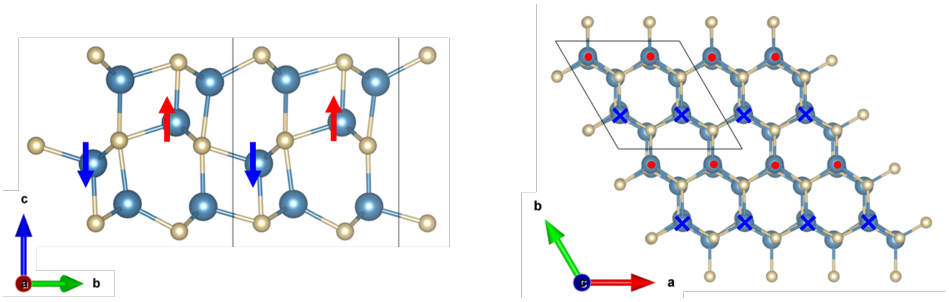

FIG. S2. Side view (left) and top view (right) of antiferroelectric 3L AlSb. Crosses and dots indicate downward and upward polarization, respectively.

III. SNAPSHOTS OF AIMD

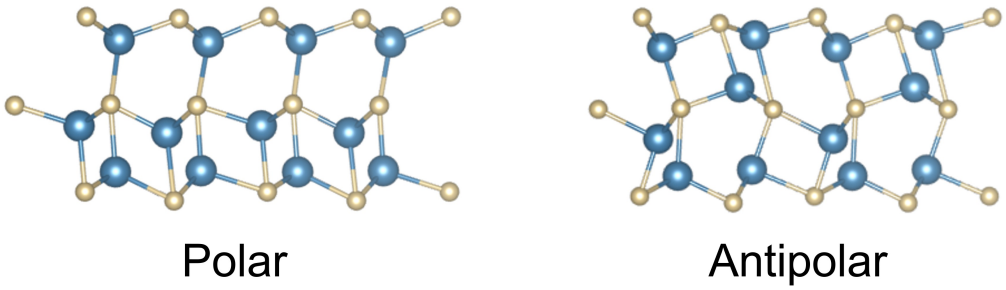

FIG. S3. Snapshots of polar (left) and antipolar (right) configurations at the end of 10 ps AIMD simulations.

IV. COMPARISON OF BAND STRCUTURES COMPUTED WITH EACBN0 AND HSE06

The comparison of the band structures computed with the hybrid functional HSE06 [1] and eACBN0 [2–4] for 3L AlSb in the ferroelectric phase is shown in Fig. S4. The eACBN0 predicts the same band dispersion as HSE06 for states over a board energy range from −8 to 2 eV but at a fractional computational cost.

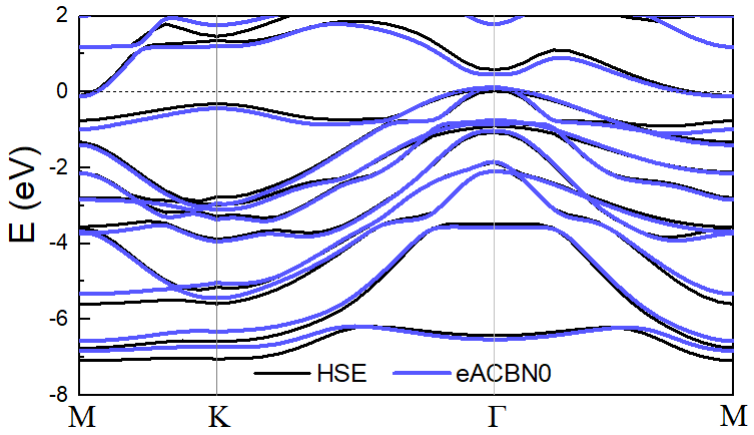

FIG. S4. Comparison of the band structures of ferroelectric 3L AlSb computed with eACBN0 and HSE06.

[1] A. V. Krukau, O. A. Vydrov, A. F. Izmaylov, and G. E. Scuseria, Influence of the exchange screening parameter on the performance of screened hybrid functionals, J. Chem. Phys. **125**, 224106 (2006).

[2] L. A. Agapito, A. Ferretti, A. Calzolari, S. Curtarolo, and M. B. Nardelli, Effective and accurate representation of extended Bloch states on finite Hilbert spaces, Phys. Rev. B **88**, 165127 (2013).

[3] S.-H. Lee and Y.-W. Son, First-principles approach with a pseudohybrid density functional for extended Hubbard interactions, Phys. Rev. Research **2**, 043410 (2020).

[4] N. Tancogne-Dejean and A. Rubio, Parameter-free hybridlike functional based on an extended Hubbard model: DFT+U+V, Phys. Rev. B **102**, 155117 (2020).