Native Point Defects in Antiperovskite Ba_3SbN: Promising Semiconductor for Photovoltaics

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Figure S1. Atomic structures of the vacancies in the neutral state.

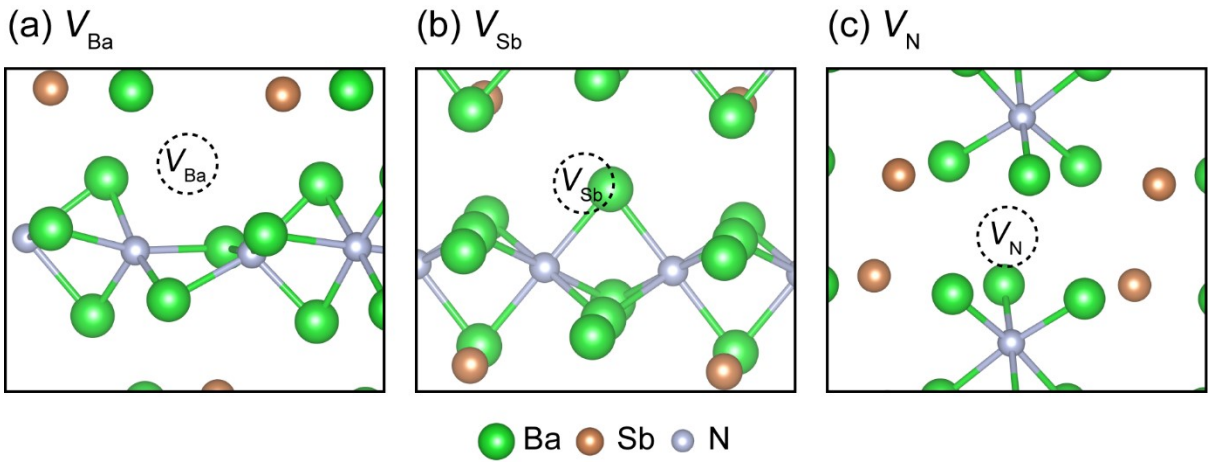


Figure S2. Atomic structures of the interstitials in the neutral state.

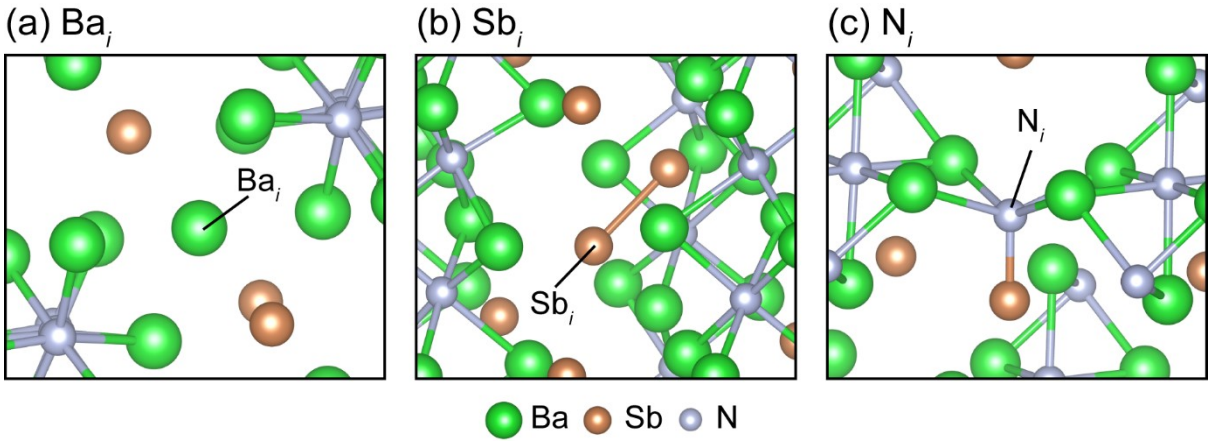


Figure S3. Atomic structures of the antisites in the neutral state.

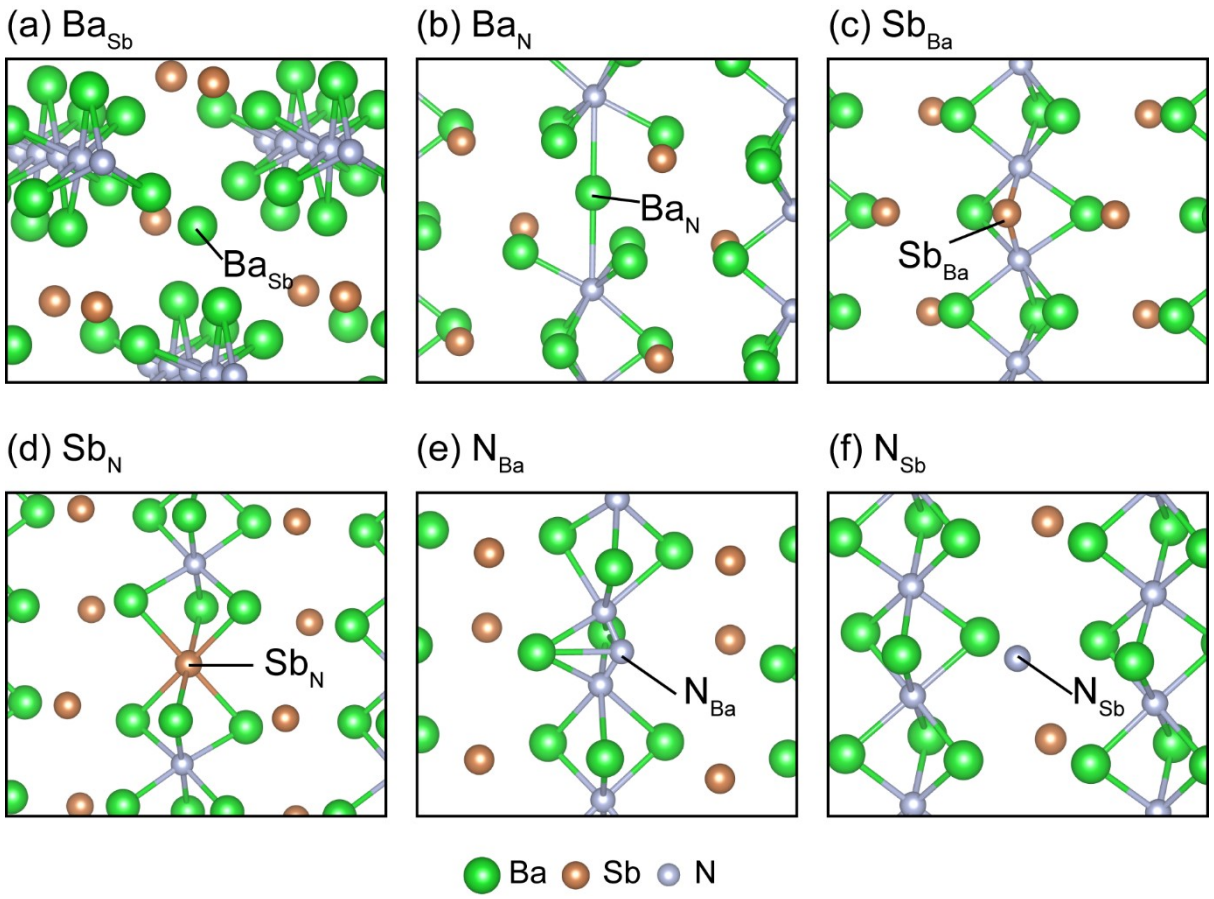
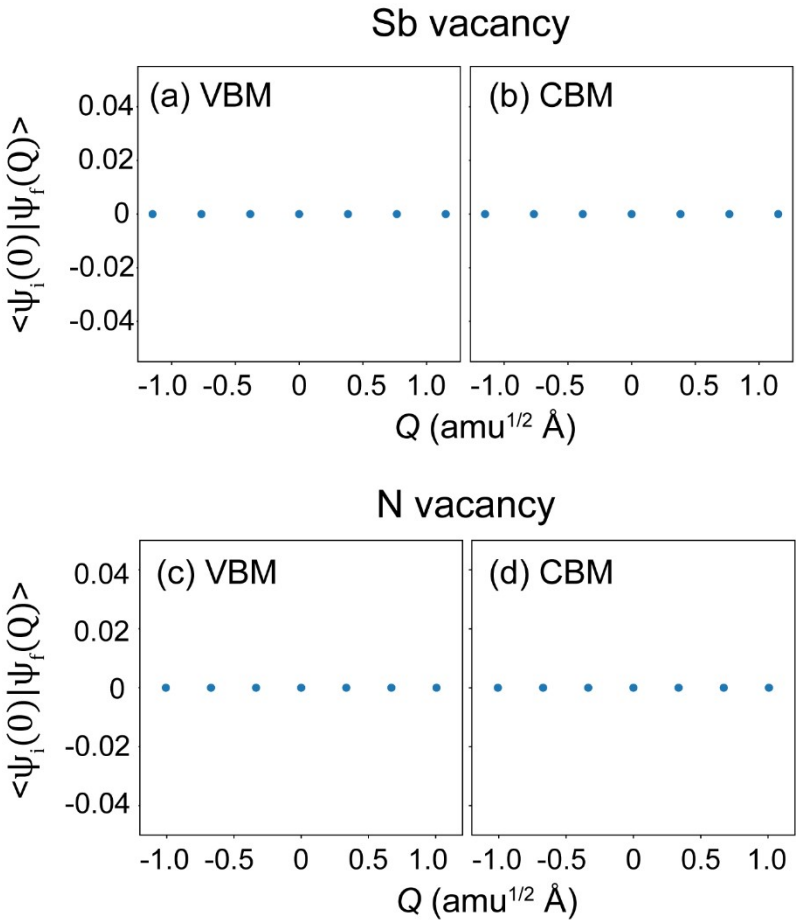


Figure S4. Overlap matrix as a function of Q in V_{Sb}-containing supercell [(a) for VBM and (b) for CBM] and V_N-containing supercell [(c) for VBM and (d) for CBM]. Here, the initial state ψ_i is the perturbed band-edge states (VBM or CBM), while the final state ψ_f is the localized



defect state.

Note that a single electron-phonon coupling matrix element W_{if} is given by:

$$W_{if} = \langle \psi_i \left| \partial \hat{H}/\partial Q \right| \psi_f \rangle,$$

where $\hat{H}$ is the Hamiltonian operator of the system. As a first-order approximation, this matrix element can be evaluated by:

$$W_{if} \approx (\epsilon_f - \epsilon_i) \langle \psi_i \left| \partial \psi_f/\partial Q \right\rangle,$$

where ϵ_f and ϵ_i is the eigenvalue of the final and initial states, respectively. $\langle \psi_i \left| \partial \psi_f/\partial Q \right\rangle$ can be calculated from the slope of the overlap matrix versus Q curve. As shown in Fig S4, the slope of the overlap matrix is negligible for both V_{Sb} and V_N defects.