Supporting Information

Theoretical Insights on the Defect Performance in Wide

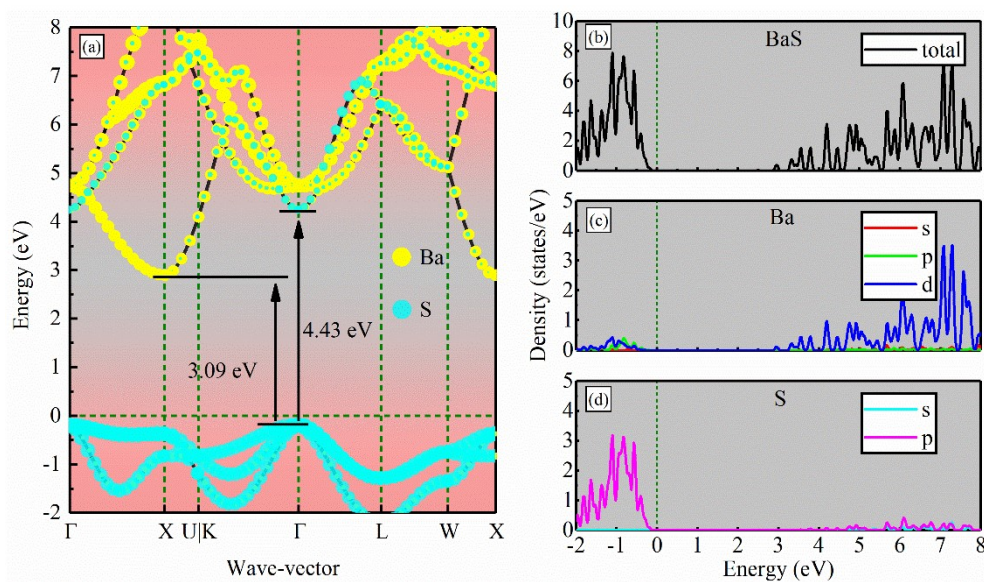# Bandgap Semiconductor BaS

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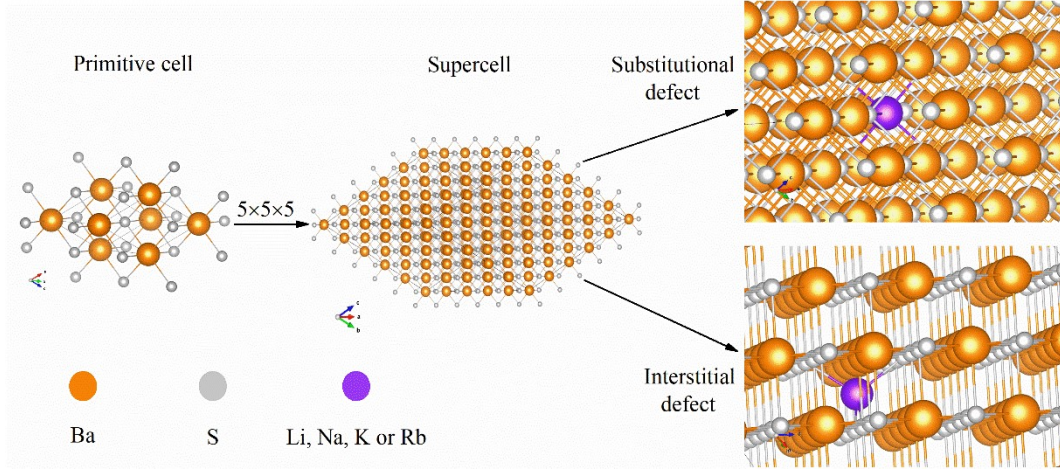of Physics, China Three Gorges University, Yichang, 443002, China

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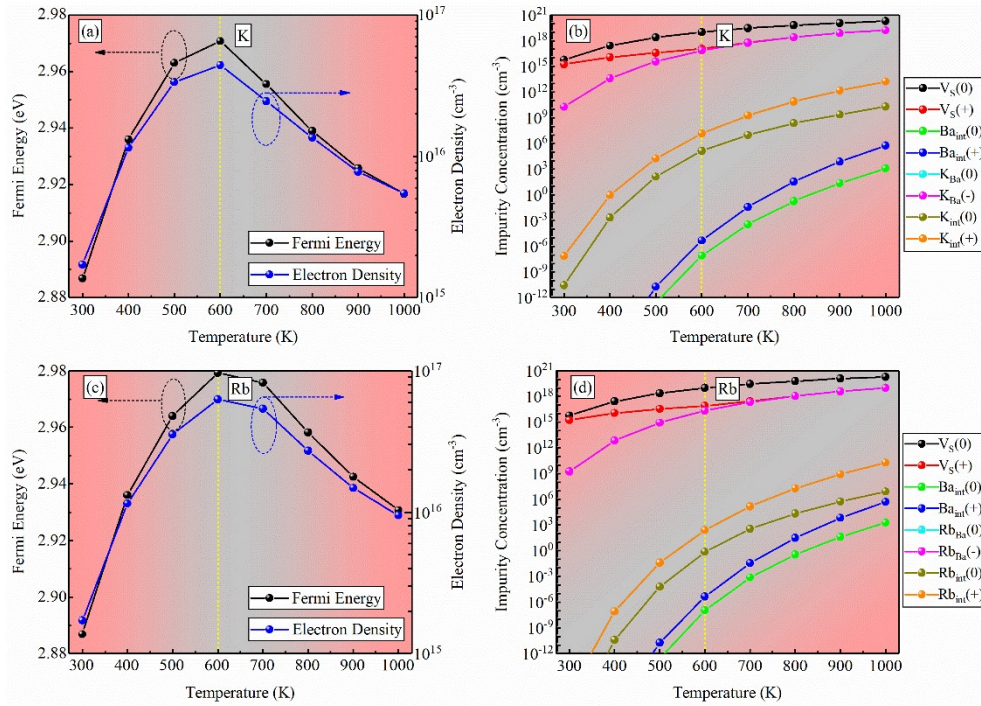430074, China

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Fig. S1 HSE06-calculated (a) projected band structure and (b) density of states of BaS are plotted.

The Fermi energy is set to 0 eV.

Fig. S2 The construction process of defective structures is plotted, where Ba, S and impurities (Li, Na, K, and Rb) atoms are marked as orange, light grey, and purple, respectively.

Fig. S3 After quenching from different T_G to room temperature, (a) ((c)) the Fermi energy positions and electron density, as well as (b) ((d)) impurity concentrations for K (Rb)-doped BaS systems under Ba-rich growth conditions are depicted. The yellow dotted lines indicate the peak value where the Fermi energy and electron density reach maximum.
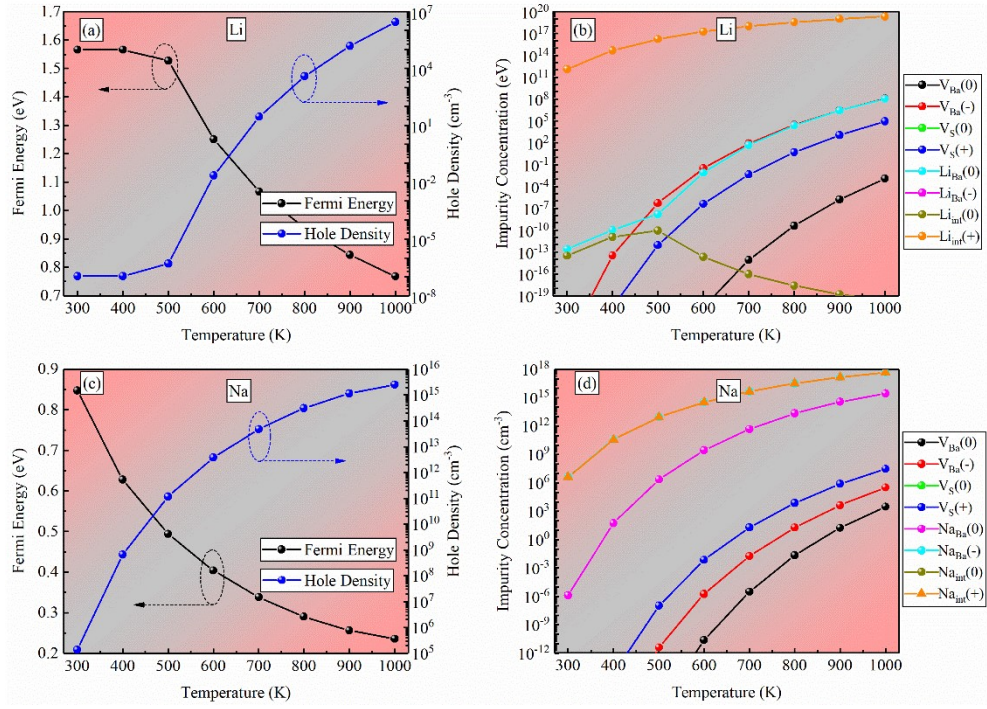
Fig. S4 After quenching from different T_G to room temperature, (a) ((c)) the Fermi energy positions and hole density, as well as (b) ((d)) impurity concentrations in Li (Na)-doped BaS systems under S-rich growth conditions are depicted.