Strain-Induced Corrugation and Its Impact on Electronic and Optical Properties of hBN-GaS, -GaSe, and -InS heterostructures

Supplementary Material

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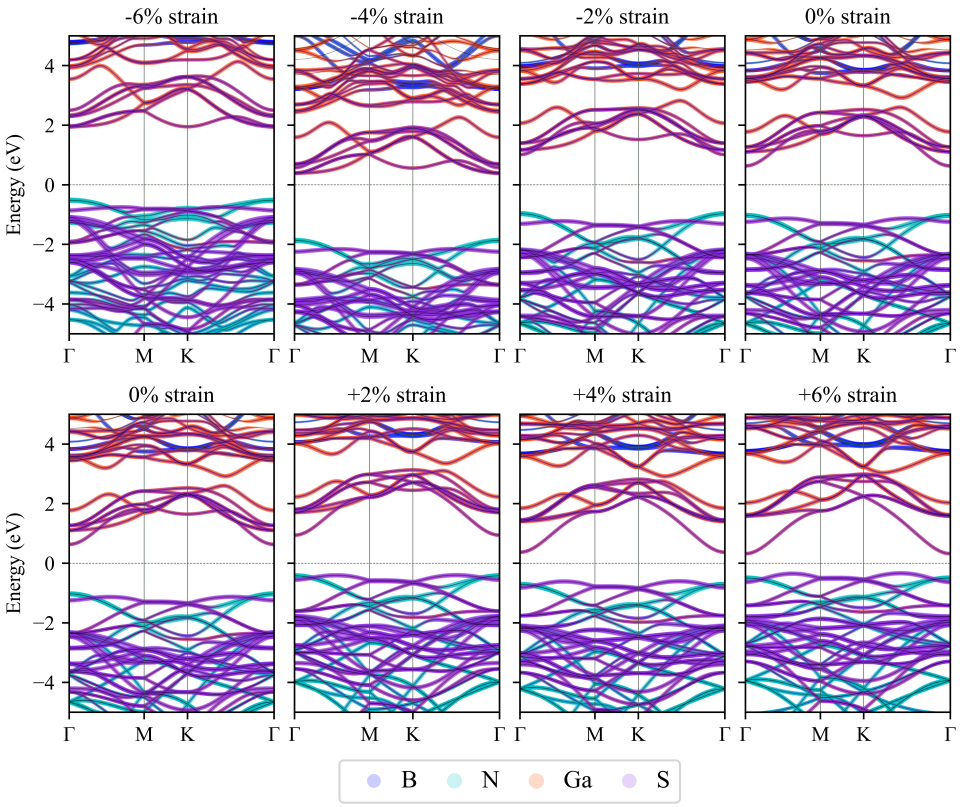

Fig. 1 Projected band structure of hBN/GaS for strain values in range from -6%, to +6%. The line width is proportional to the contribution of different atoms/states.

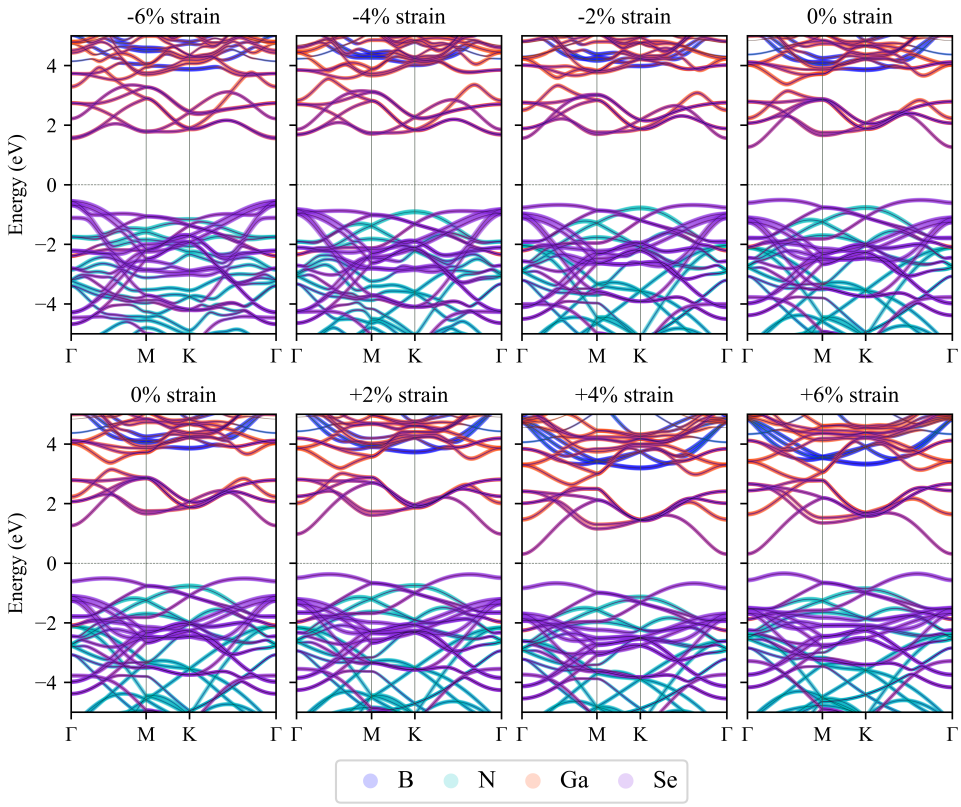

Fig. 2 Projected band structure of hBN/GaSe for strain values in range from -6%, to +6%. The line width is proportional to the contribution of different atoms/states.

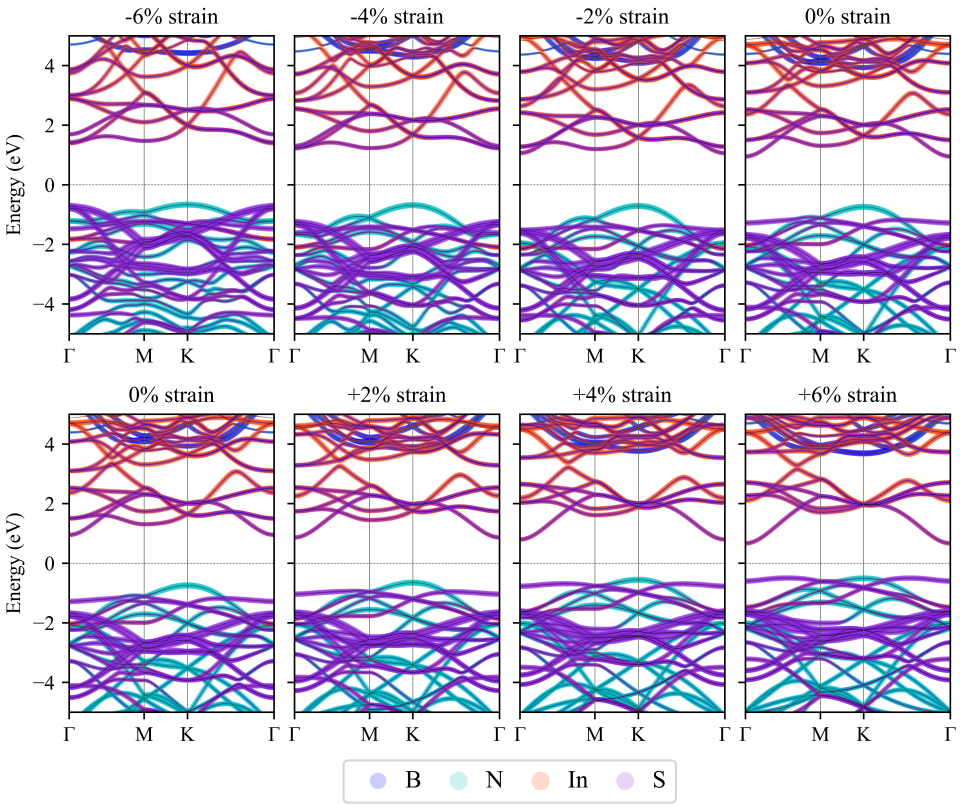

Fig. 3 Projected band structure of hBN/InS for strain values in range from -6%, to +6%. The line width is proportional to the contribution of different atoms/states.

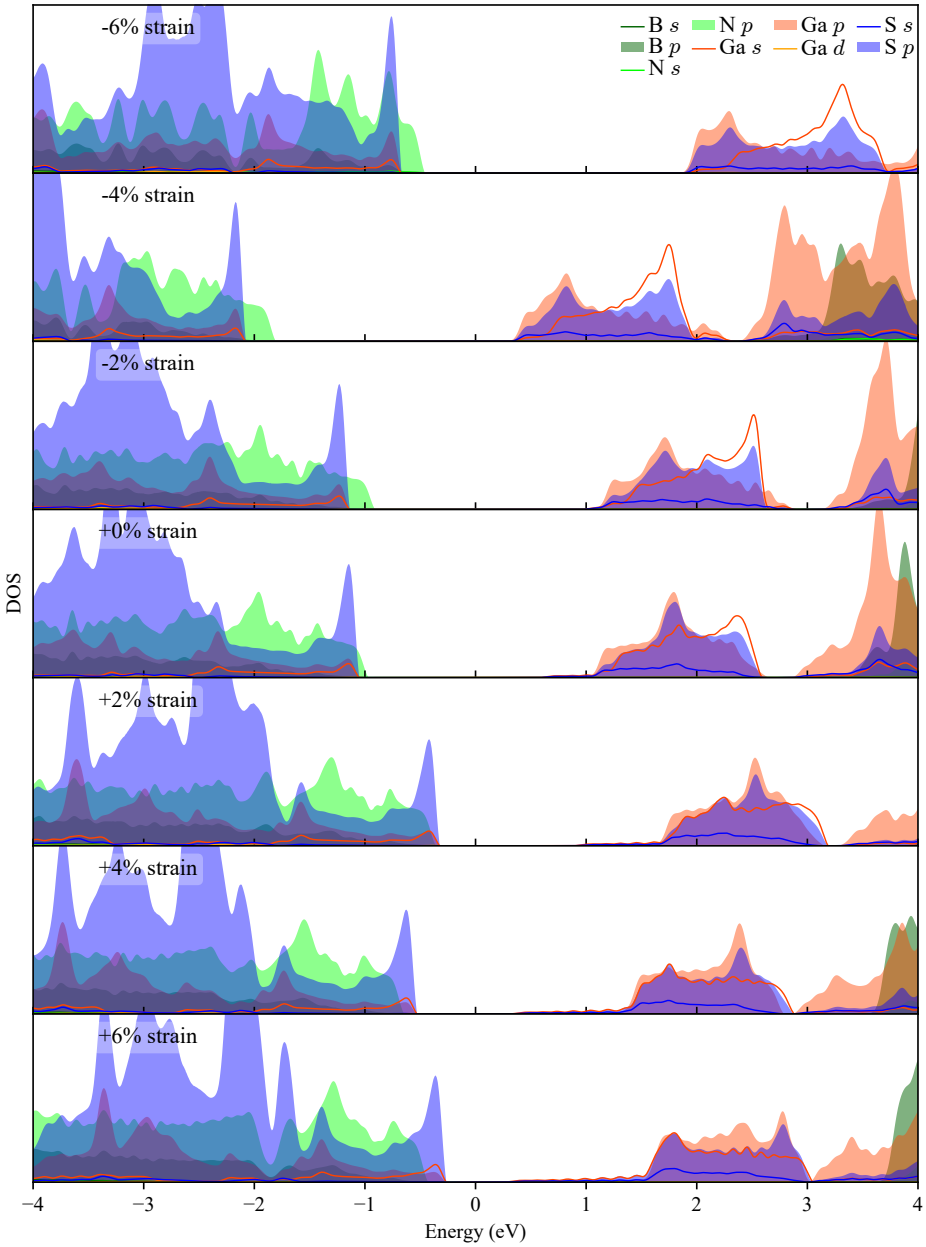

Fig. 4 Projected density of states (PDOS) of hBN/GaS HSs calculated for applied strain values in range from -6%, to +6%. Contribution from different atoms and states are represented as shown in legend.

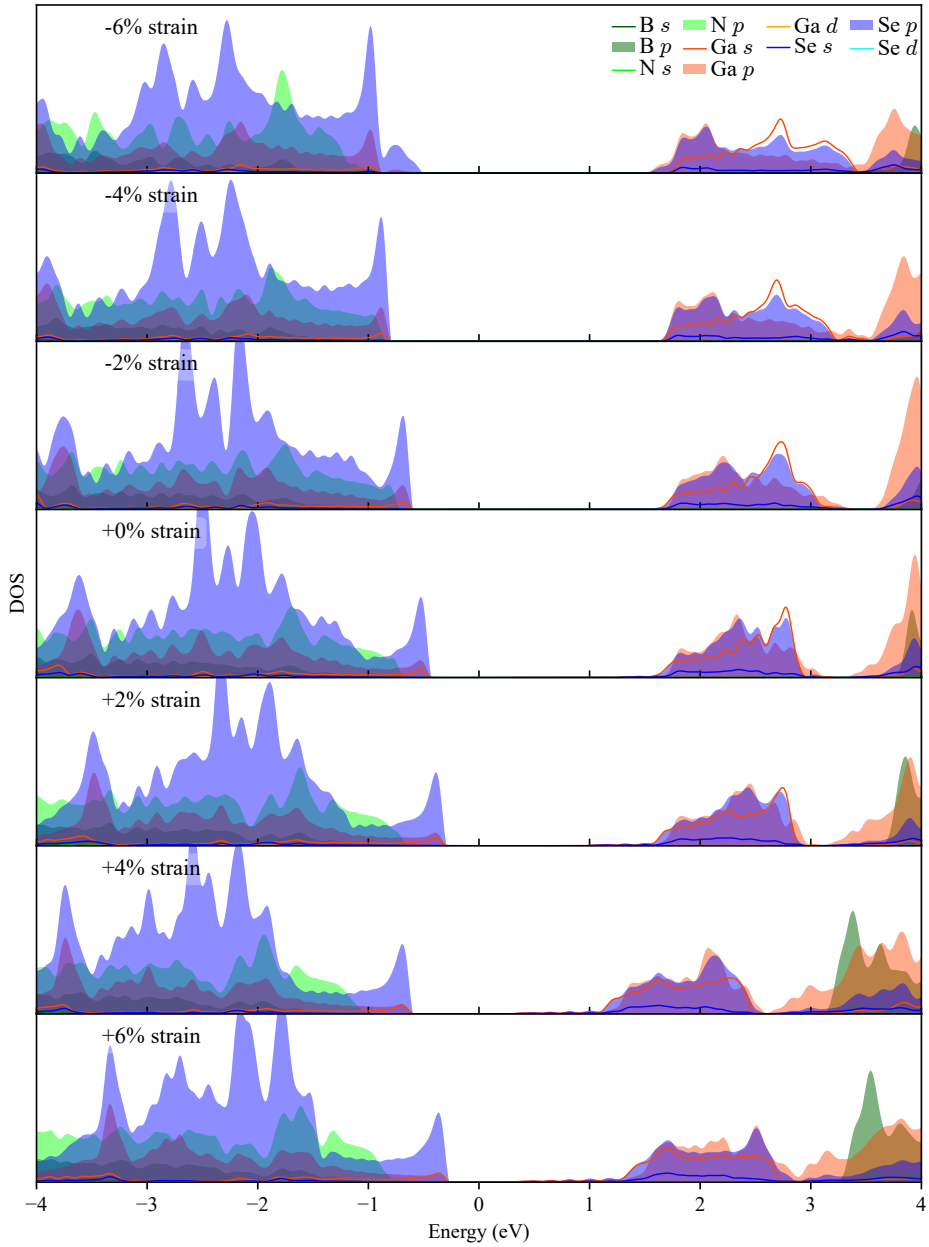

Fig. 5 Projected density of states (PDOS) of hBN/GaSe HSs calculated for applied strain values in range from -6%, to +6%. Contribution from different atoms and states are represented as shown in legend.

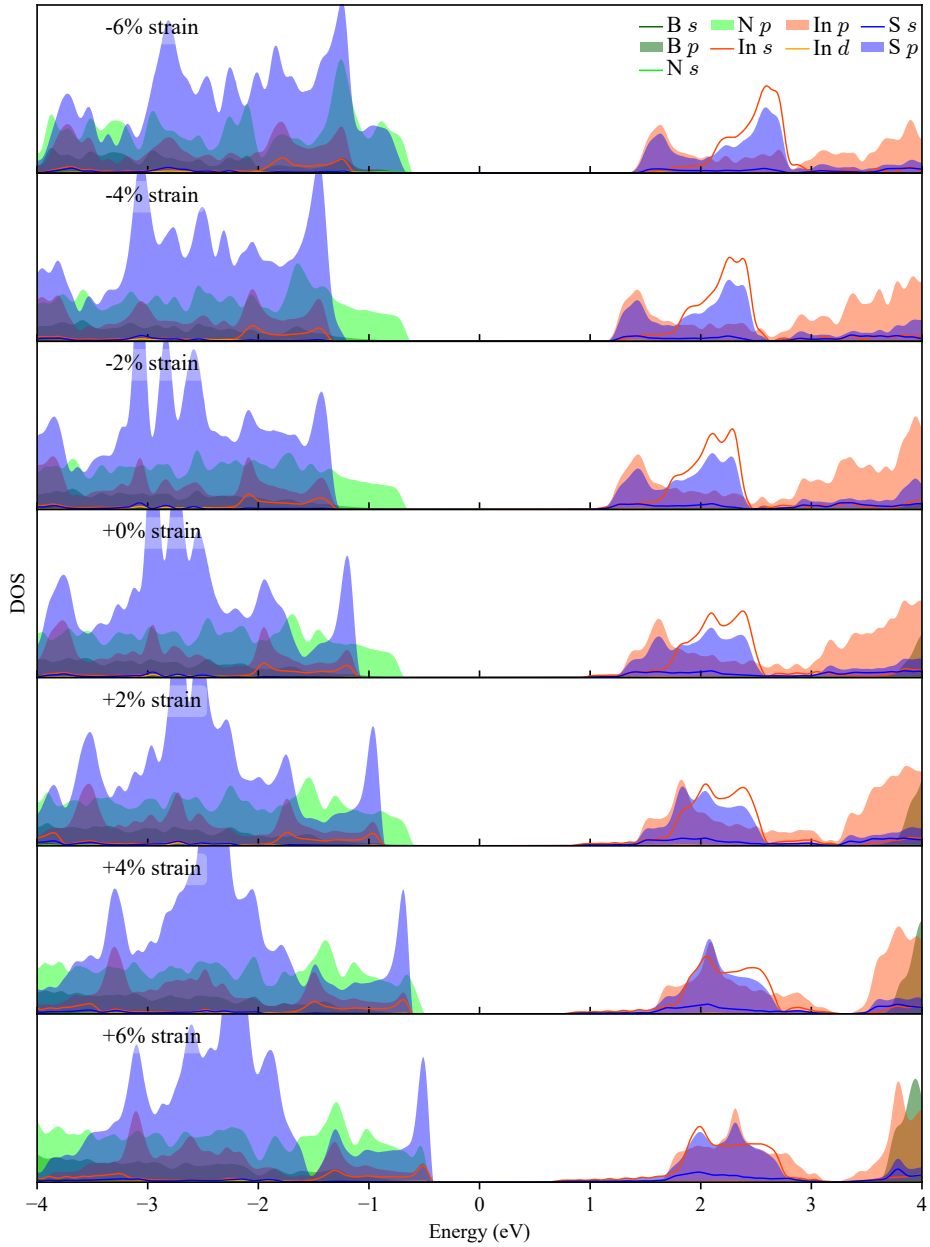

Fig. 6 Projected density of states (PDOS) of hBN/InS HSs calculated for applied strain values in range from -6%, to +6%. Contribution from different atoms and states are represented as shown in legend.