

Supplementary information for

“Ternary Pentagonal BXN (X = C, Si, Ge and Sn) Sheets with High Piezoelectricity”

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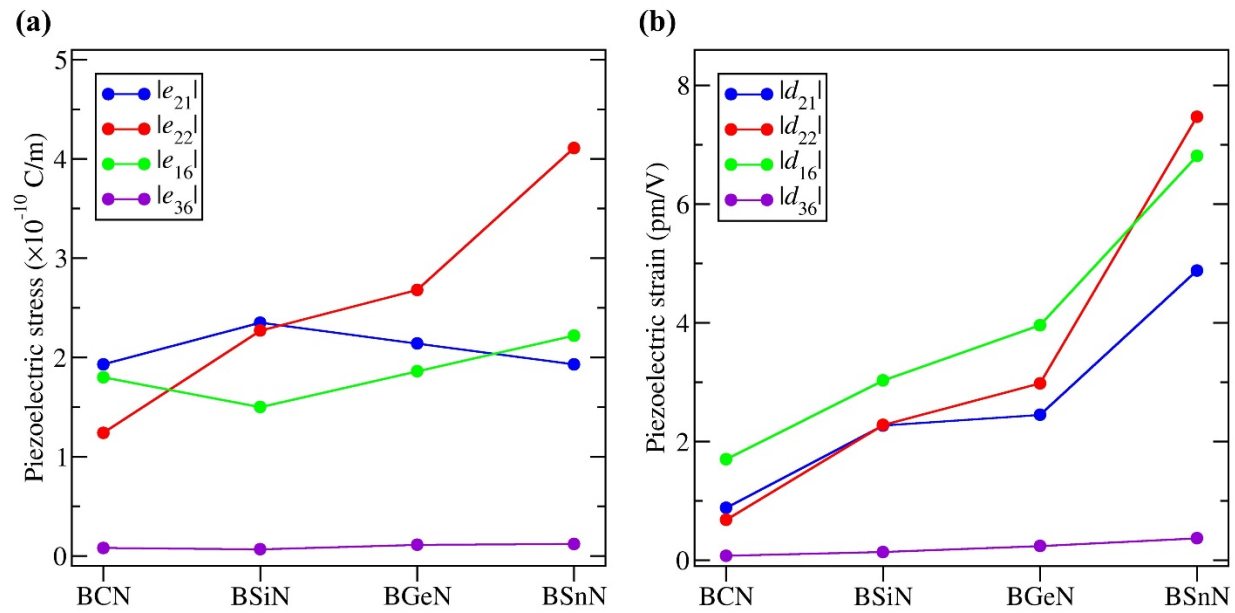


FIG S1 The (a) piezoelectric stress tensors and (b) piezoelectric strain tensors of *penta*-BXN (X=C, Si, Ge and Sn)

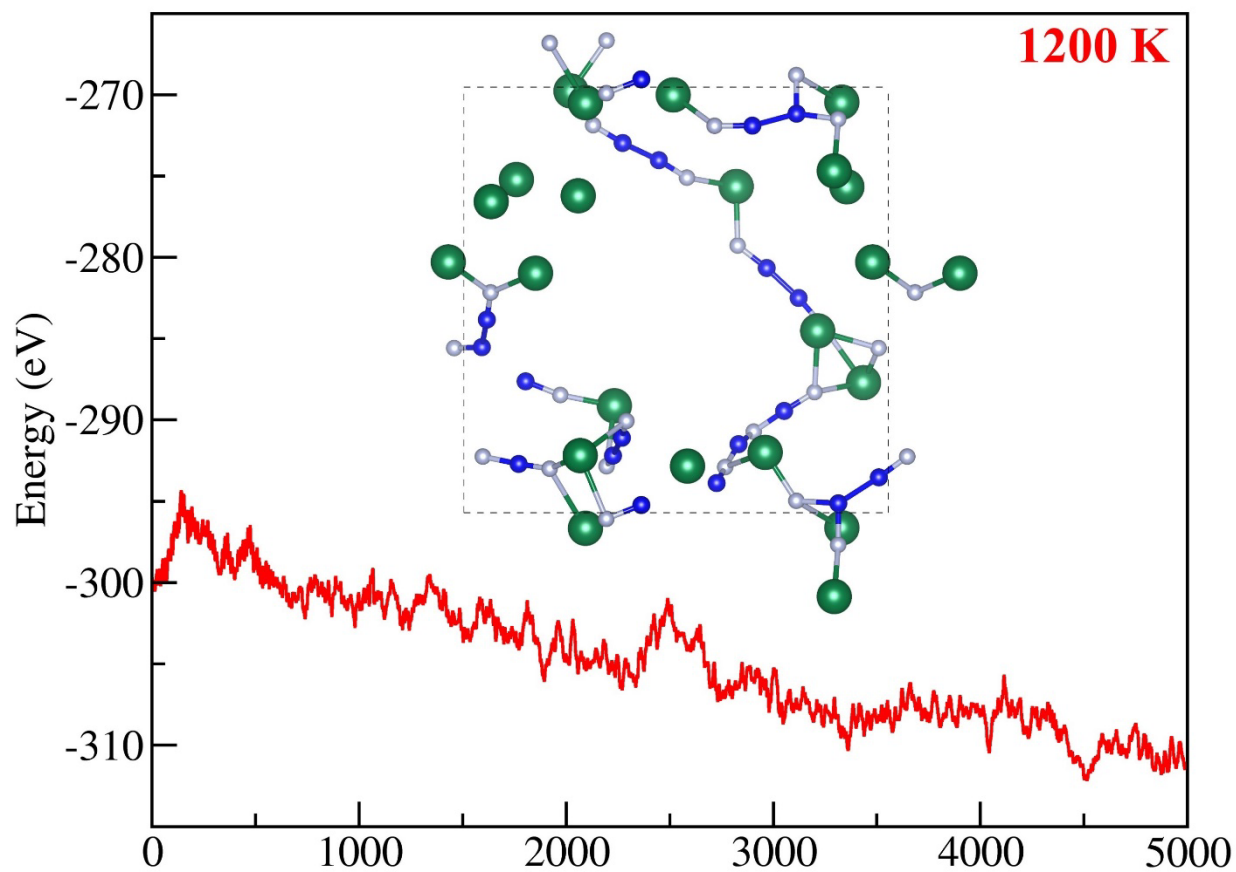


FIG S2 MD simulation of *penta*-BSnN at temperature of 1200 K

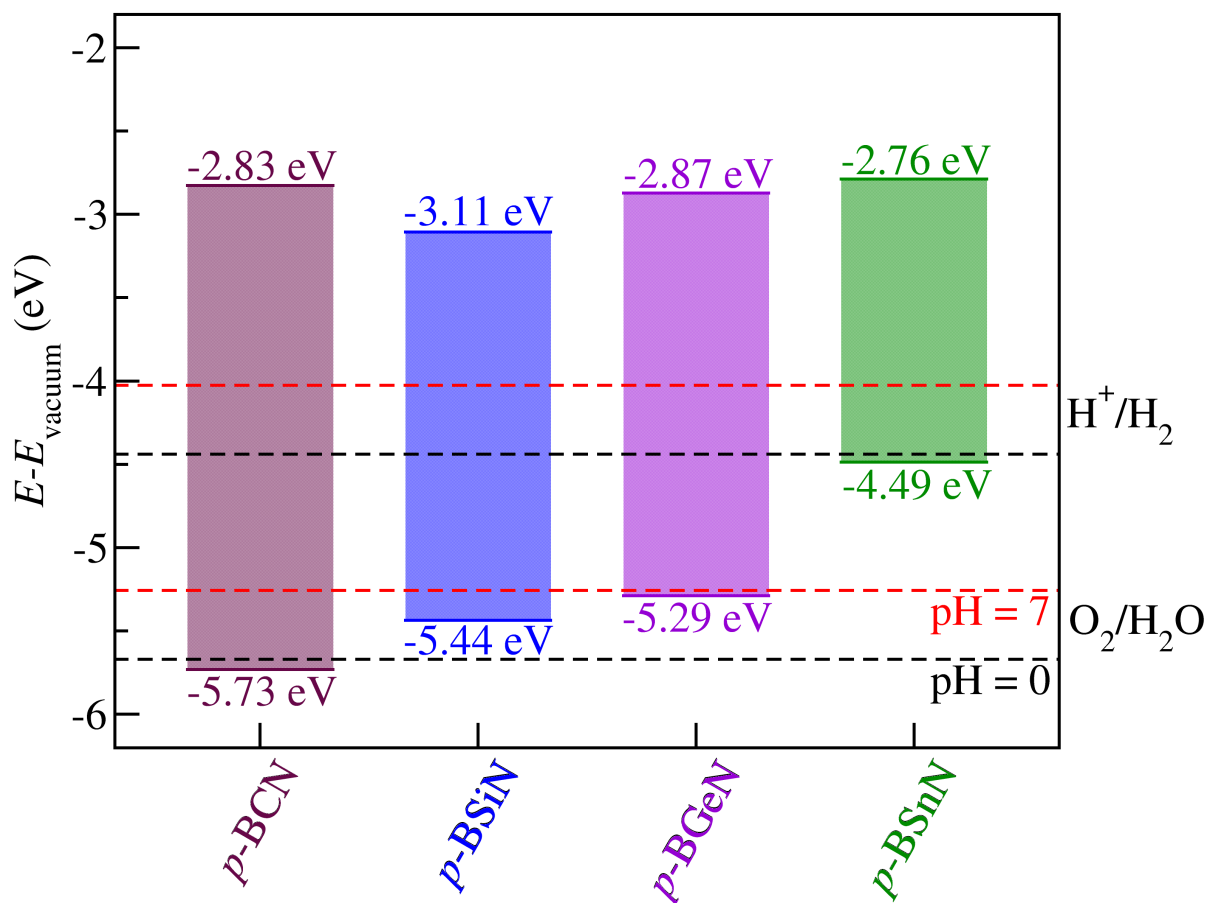


FIG S3 Band edge alignment of the ternary *penta*-BXN with relation to the redox potentials for water-splitting at $\text{pH} = 0$ (black dash line) and $\text{pH} = 7$ (red dash line).