**Supplementary Information**

**Atomic Structure and Electronic Properties of A2B2XY (A = Si-Pb, B = Cl-I, and XY = PN and SiS) Inorganic Double Helices: First Principles Calculations**

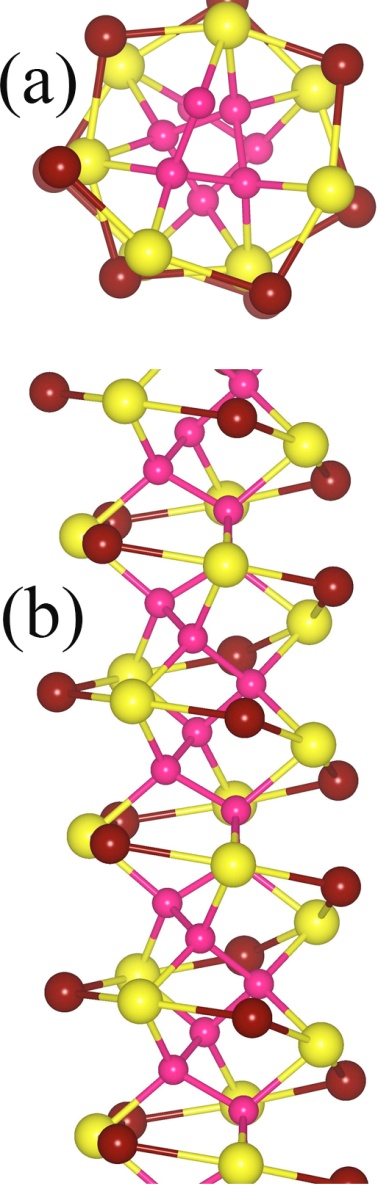
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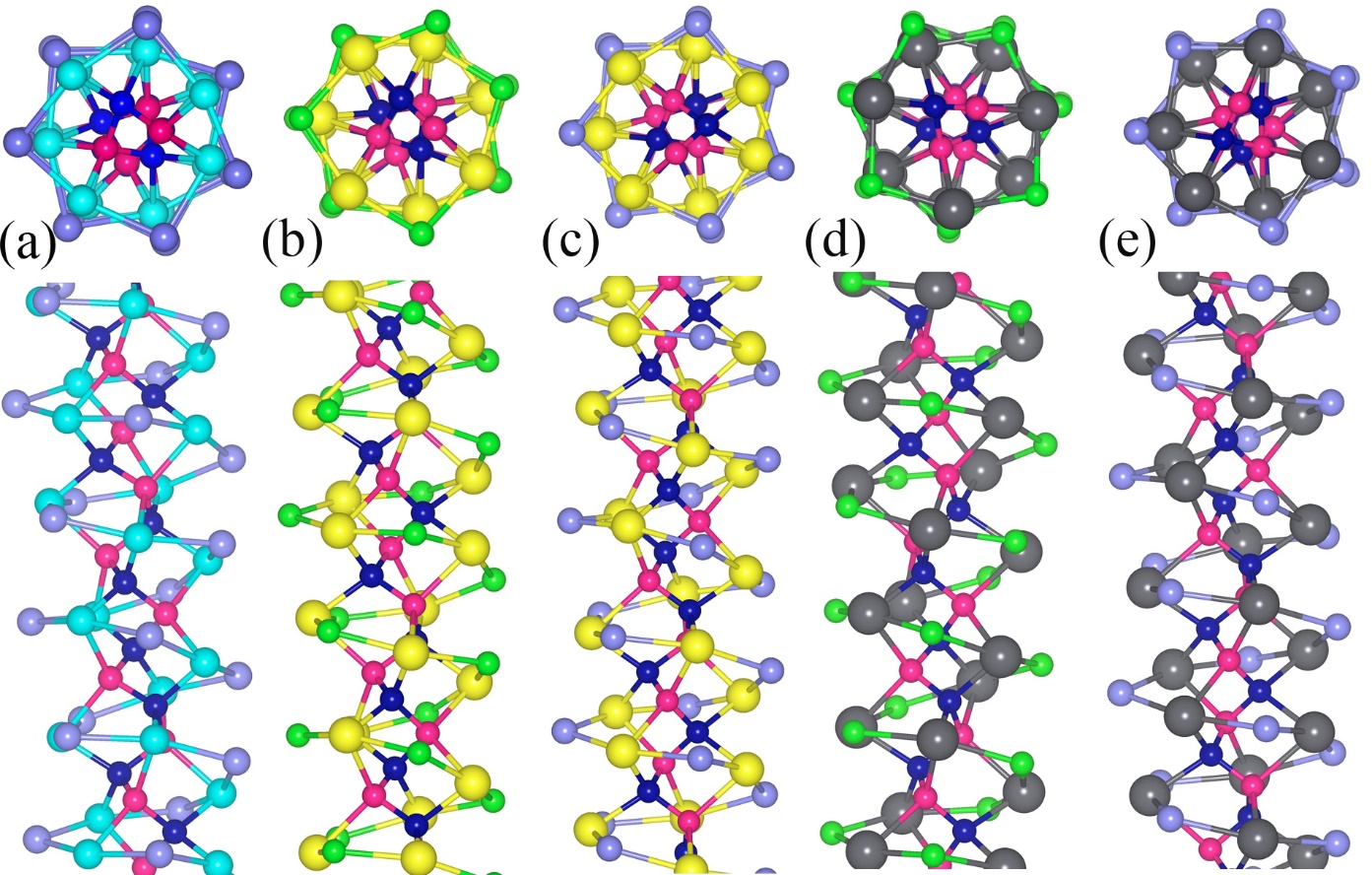
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c*Functional Materials Division- CSIR-Central Electrochemical Research Institute, Karaikudi, Tamil Nadu, India*

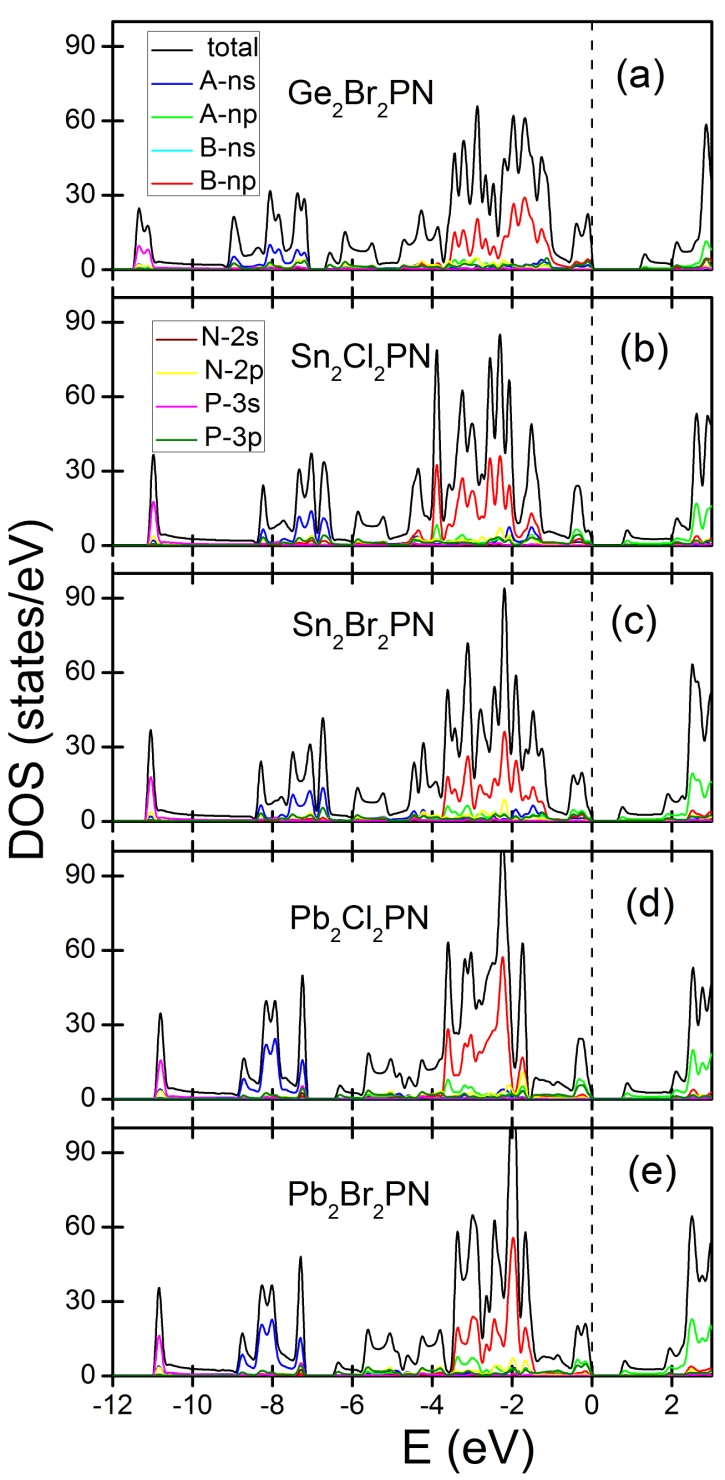
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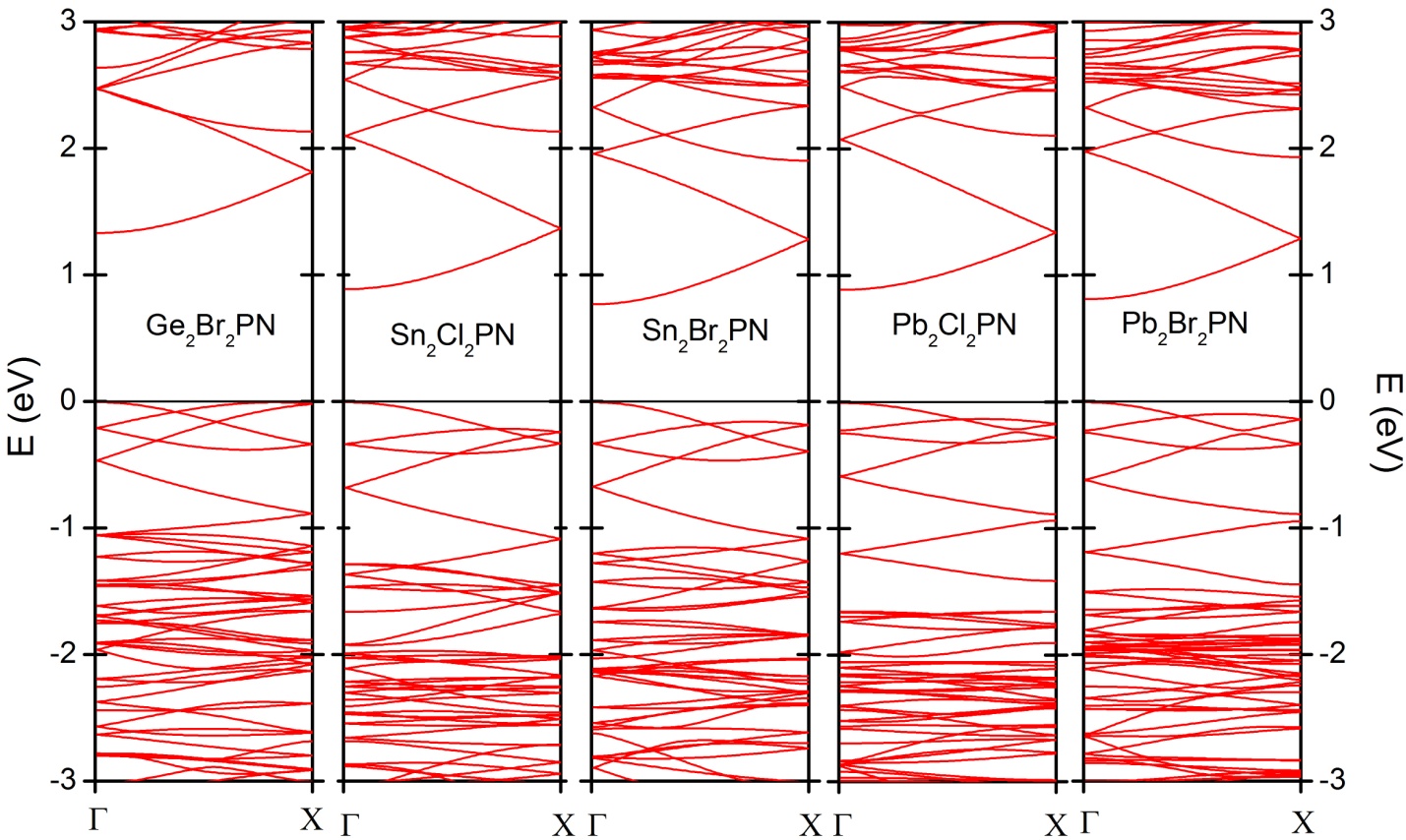
**Fig. S1.** (a) Top and (b) side views of the optimized atomic structure of SnIP double helix. Yellow, brown, and pink color balls represent Sn, I, and P atoms, respectively. P atoms form the inner helix while Sn and I atoms form the outer helix. The two helices are interconnected with each P atom tetrahedrally bonded with two neighboring P atoms in the inner helix and two Sn atoms in the outer helix. Each I atom is bonded with two neighboring Sn atoms and does not have direct interaction with p atoms in the inner helix.



**Fig. S2.** Top and side views of the optimized atomic structures of the double helices of (a) Ge2Br2PN, (b) Sn2Cl2PN, (c) Sn2Br2PN, (d) Pb2Cl2PN, and (e) Pb2Br2PN. Pink and blue balls represent the inner PN helix while cyan, yellow, grey, green, and silver balls show Ge, Sn, Pb, Cl, and Br atoms in the outer helix, respectively.



**Fig. S3.** Total and partial(angular momentum resolved)electronic densities of states of (a) Ge2Br2PN, (b) Sn2Cl2PN, (c) Sn2Br2PN, (d) Pb2Cl2PN, and (e) Pb2Br2PN double helices. The vertical broken line shows the top of the valence band which has been taken as reference for energy. One can see that the *s* states of the A atom (blue curve) lie around -7 eV to -8 eV while the 2*p* states of the B atoms (red curve) lie around -2 eV to -3 eV. There is some contribution (green curve) from the *p* orbitals of the A atoms in the valence band but larger contribution arises in the conduction band. The 3s states of P atoms lie around -11 eV.

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**Fig. S4.** Electronic band structures of Ge2Br2PN, Sn2Cl2PN, Sn2Br2PN, Pb2Cl2PN and Pb2Br2PN double helices. The top of the valence band has been taken as reference for energy.