Supporting material for: High density nanopore 3-triangulene kagome lattice

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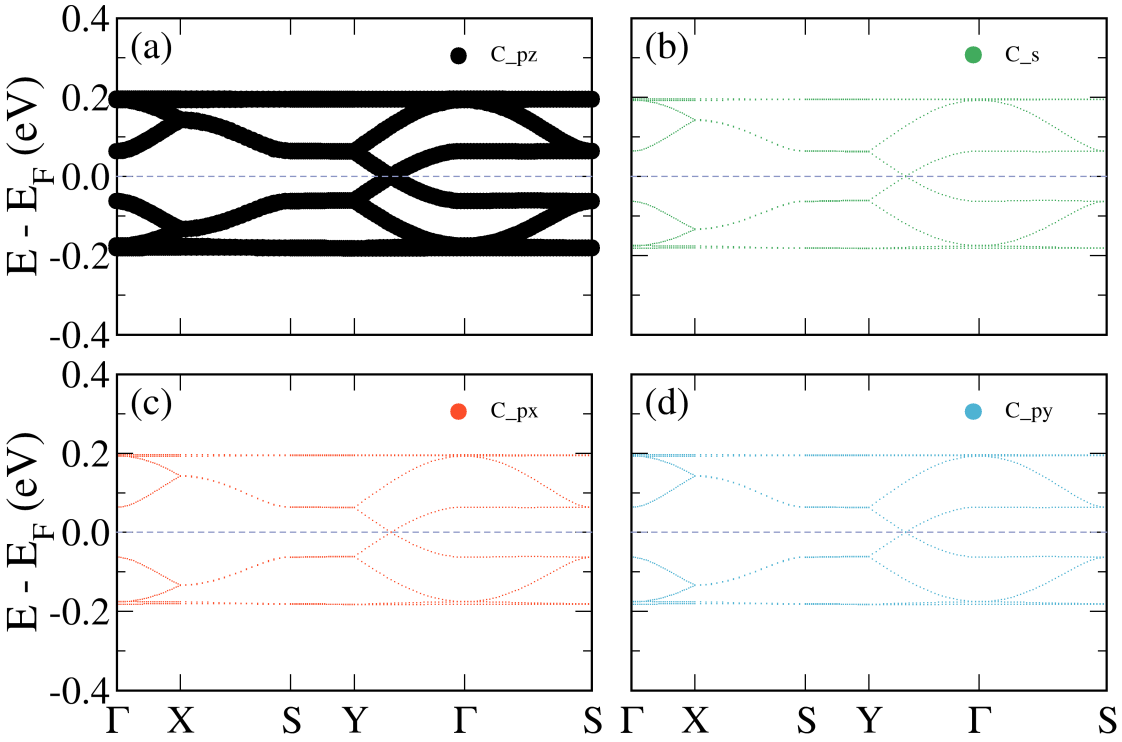

Fig. S1 Projected band structure for carbon orbitals of 3-triangulene kagome pristine, (a) C-p_z, (b) C-s, (c) C-p_x and (d) C-p_y.

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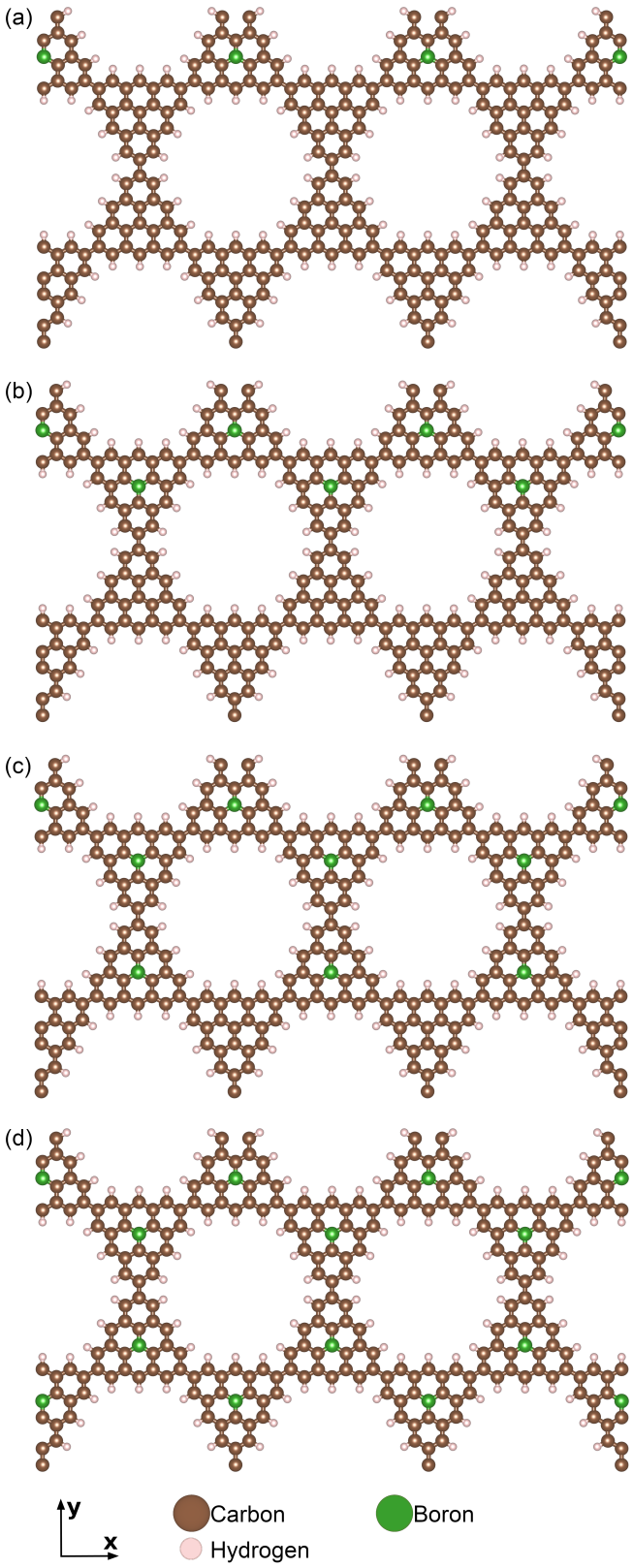

Fig. S2 Optimized geometry of the scattering region of the transport device of B-doped 3-triangulene kagome: (a) 1B-doped, (b) 2B-doped, (c) 3B-doped and (d) 4B-doped .

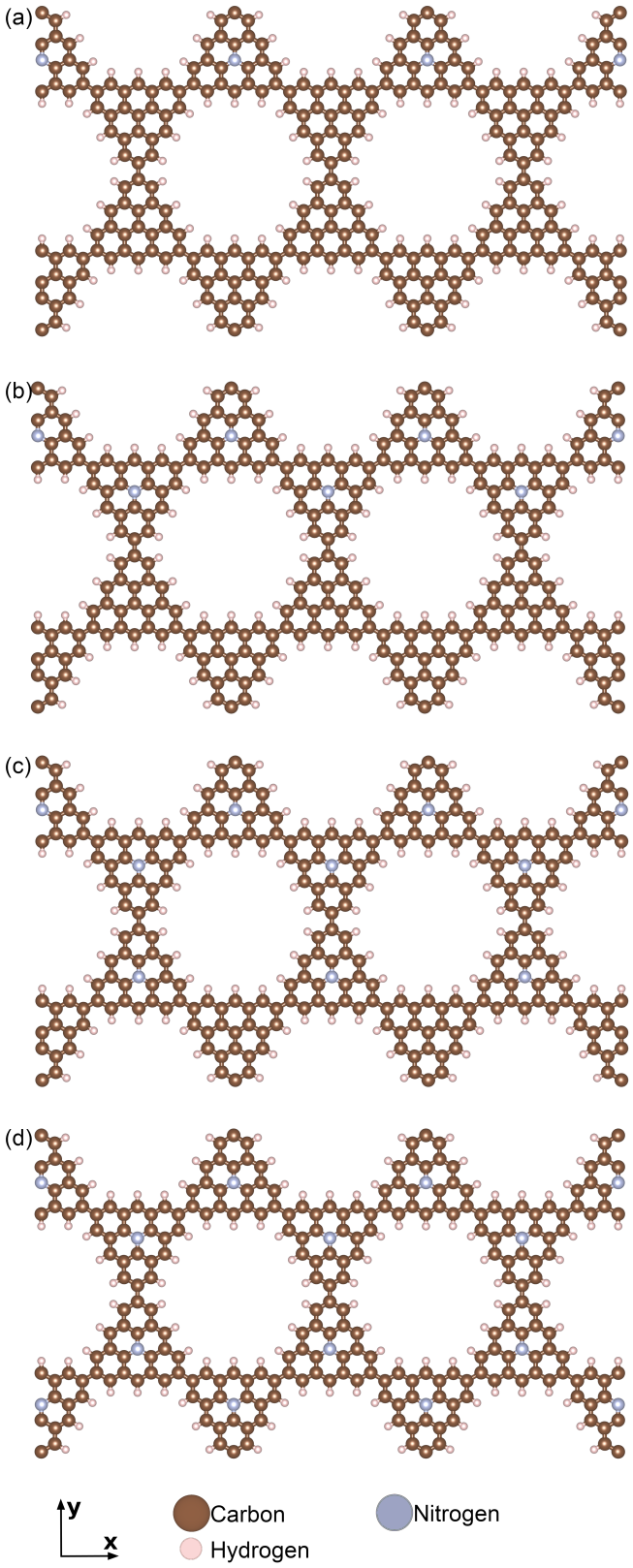

Fig. S3 Optimized geometry of the scattering region of the transport device of N-doped 3-triangulene kagome: (a) 1N-doped, (b) 2N-doped, (c) 3N-doped and (d) 4N-doped.

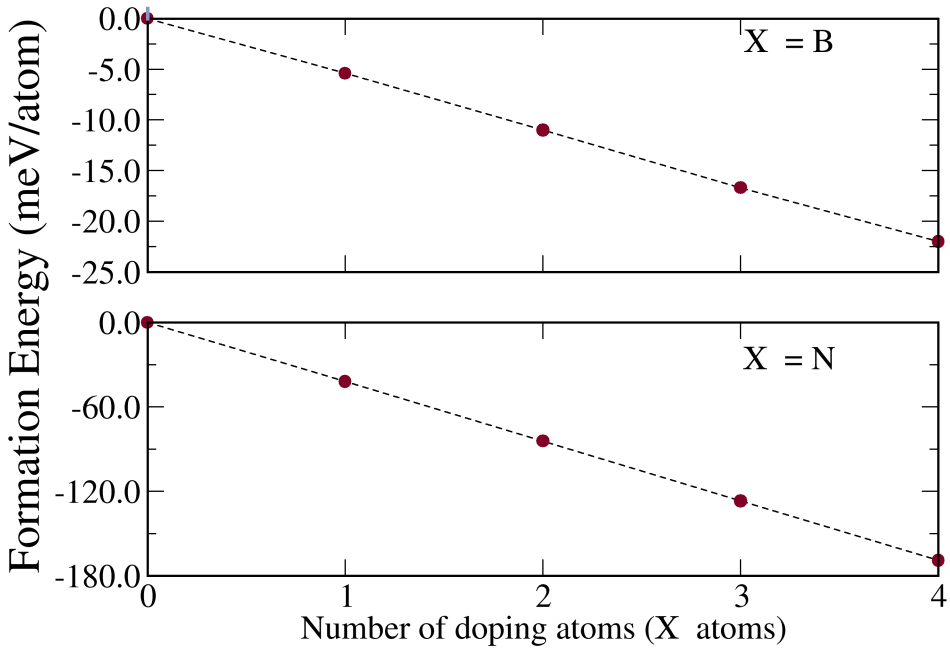

Fig. S4 Formation energy per atoms for the doped systems.

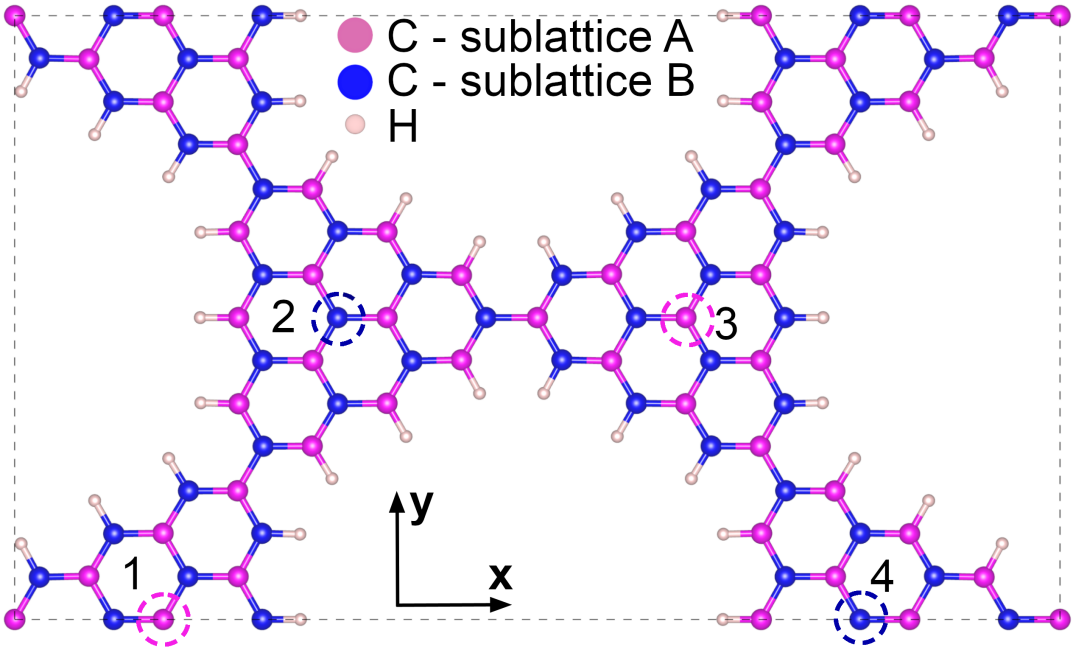

Fig. S5 Rectangular unit cell of 3-triangulene kagome crystal, where doping sites (sublattice A) are indicated by 1 and 3 (the magenta dashed circles), whereas sites (sublattce B) by 2 and 4 (blue dashed circles). In the figure, carbon atoms of sublattice A are magenta, while those of sublattice B are blue. Hydrogen atoms are light pink. So for the concentration of two dopants, the doping occurs in the same sublattice to the combinations of 1 and 3 sites or 2 and 4 sites. For the combinations of 1 and 2, 1 and 4, 2 and 3, and finally 3 and 4, the doping occurs in different sublattices. The physical implicancies of these different doping schemes where discussed in the main text.

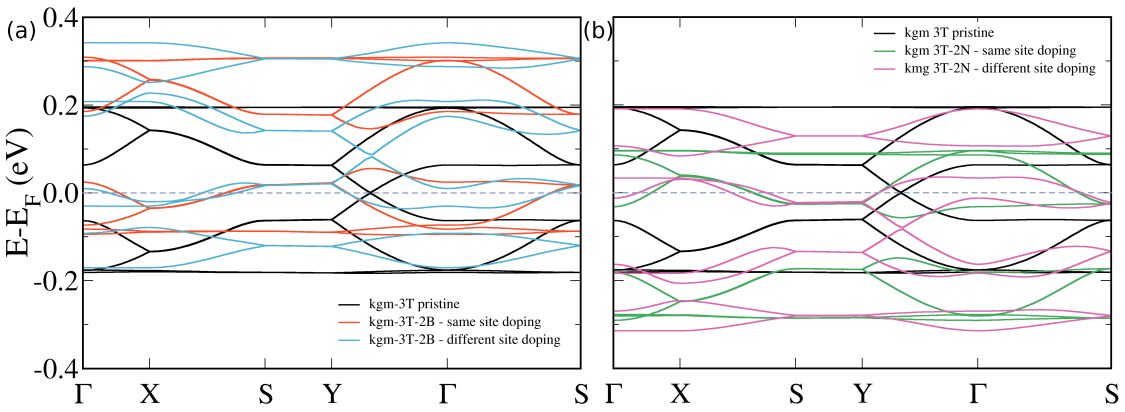

Fig. S6 The pristine 3-triangulene kagome band structure is represents by black solid lines. (a) 3-triangulene kagome with 2 boron atoms doped in the same sublattice (orange solid lines) and with 2 boron atoms doped in the different sublattice (cyan solid lines) and (b) 3-triangulene kagome with 2 boron atoms doped in the same sublattice site (green solid lines) and with 2 nitrogen atoms doped in the different sublattice site (magenta solid lines).

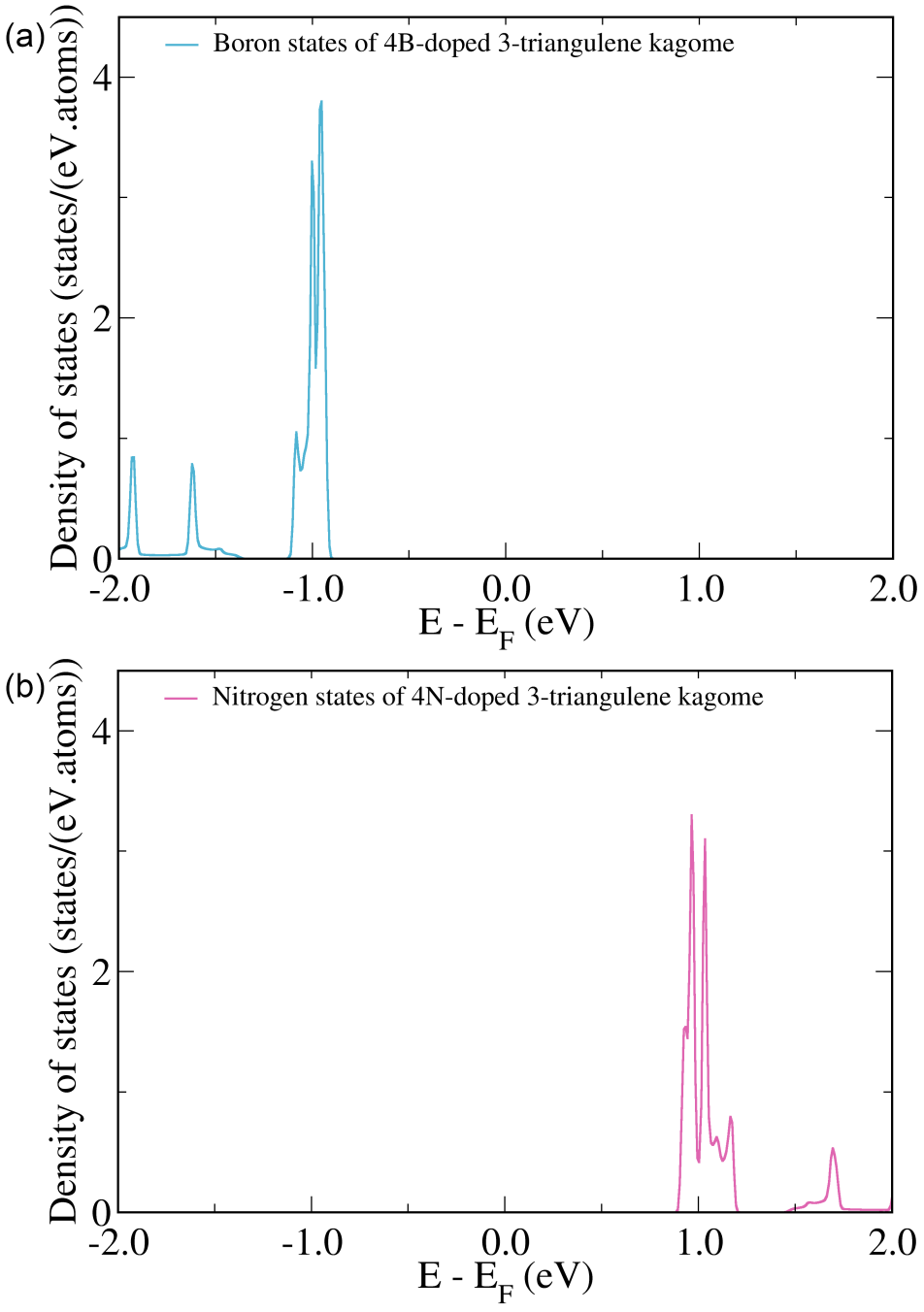

Fig. S7 Projected Density of States for (a) boron atoms at 4B-doped 3-triangulene kagome and (b) nitrogen atoms at 4N-doped 3-triangulene kagome.