Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information (SI): **Electronic and Optical Properties of Two-Dimensional Heterostructures and Heterojunctions between Doped-Graphene and C- and N-containing Materials**

A. Bafekry [a,b*] , D. Gogova [c] , Chuong V. Nguyen [d] , M. M. Fadlallah [e] , Mitra Ghergherehch[f] , M. Faraji[g] , S. A. H. Feghhi[b] , M. Oskoeian [h]

[a]Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium
[b]Department of Radiation Application, Shahid Beheshti University, Tehran, Iran
[c]Department of Physics, University of Oslo, P.O. Box 1048, Blindern, Oslo, Norway
[d]Department of Materials Science and Engineering, Le Quy Don Technical University, Hanoi, Vietnam
[e]Department of Physics, Faculty of Science, Benha University, 13518 Benha, Egypt
[f]College of Electronic and Electrical Engineering, Sungkyun Kwan University, Suwon, Korea
[g]Micro and Nanotechnology Graduate Program, TOBB University of Economics and Technology, Sogutozu Caddesi No 43 Sogutozu, 06560, Ankara, Turkey
[h] Department of physics, University of Guilan, 41335-1914 Rasht, Iran

*To whom correspondence should be addressed.
bafekry.asad@gmail.com

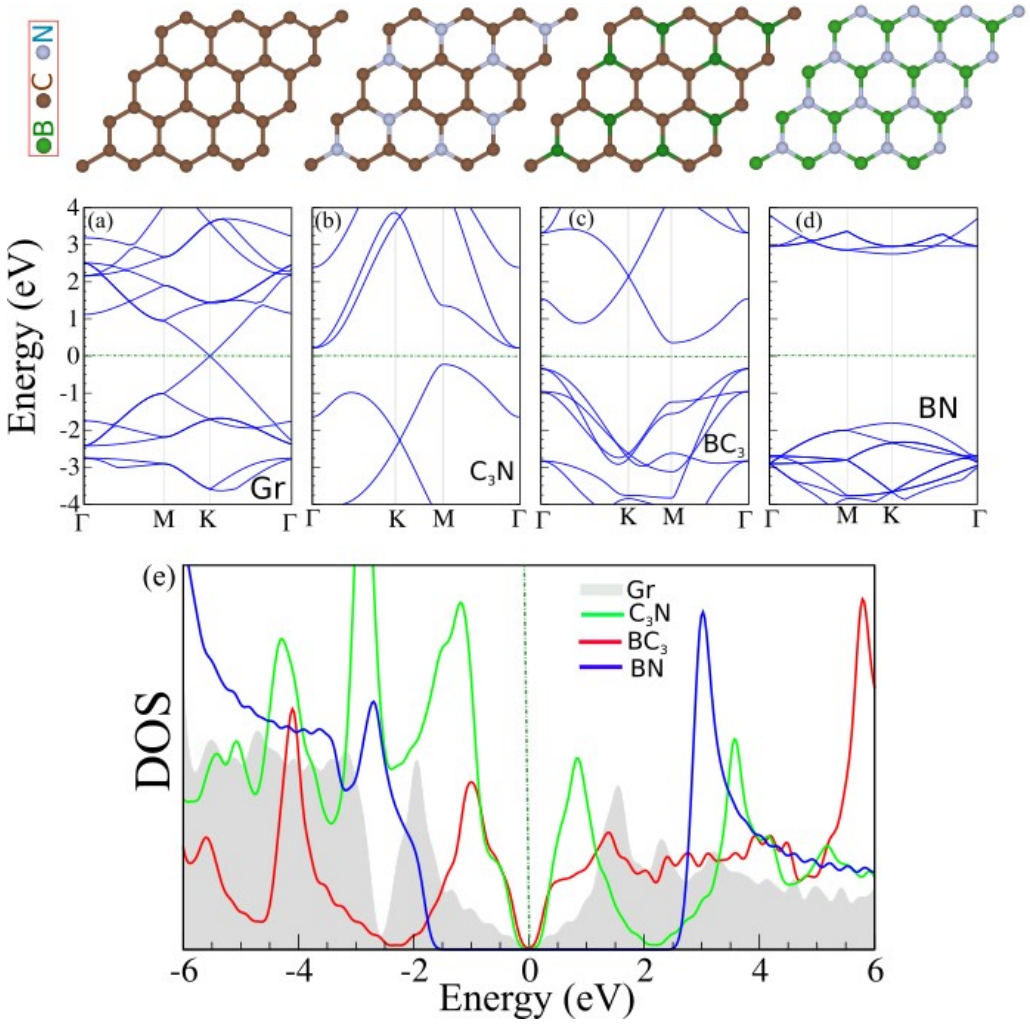

Fig. S1. Optimized structures (top) and band structures (bottom) of (a) graphene, (b) C_3N , (c) BC_3 and (d) h-BN monolayers, (e) density of states (DOS) of these monolayers. The energy is calculated relative to the Fermi energy.

*To whom correspondence should be addressed.
bafekry.asad@gmail.com

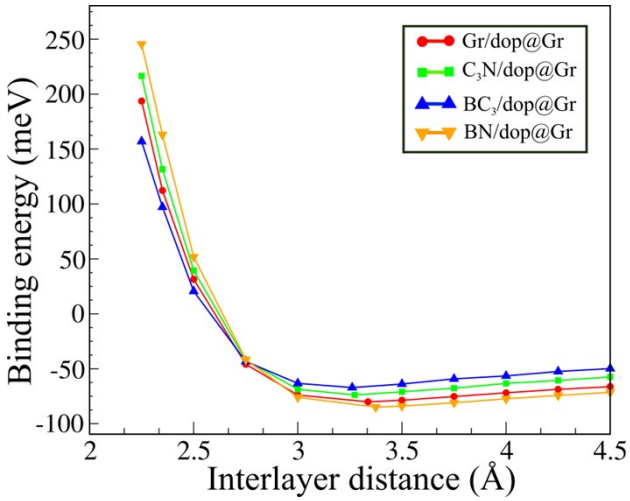

Fig. S2. The dependence of the binding energy on the interlayer distance for Gr/dop@Gr, C_3N/dop@Gr, BC3/dop@Gr and BN/dop@Gr HTSs.

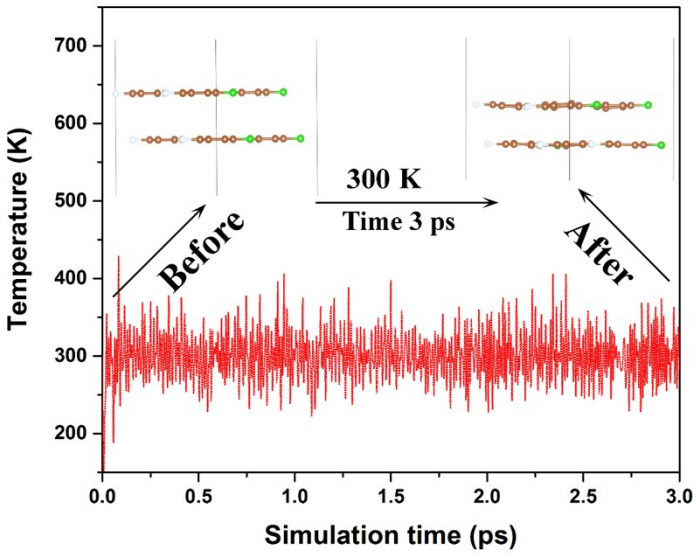

Fig. S3. Ab initio molecular dynamics (AIMD) for C_3N/dop@Gr at 300 K. The top view of optimized structure at 300 K are shown in the inset.

*To whom correspondence should be addressed.
bafekry.asad@gmail.com

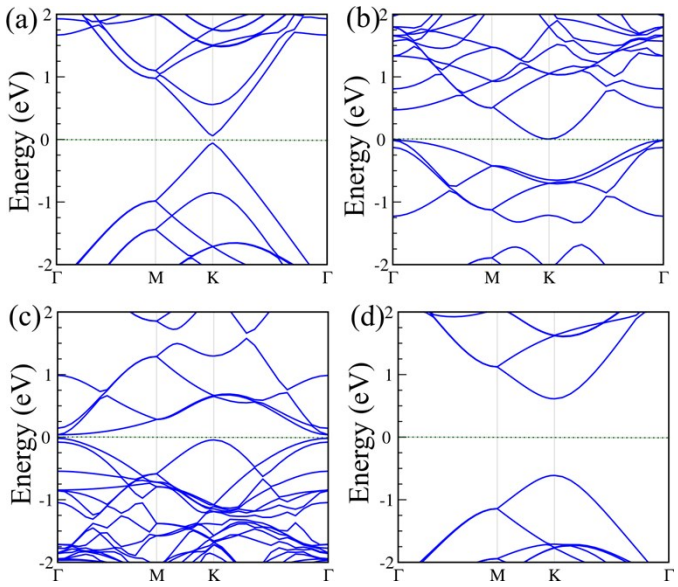

Fig. S4 The electronic band structure of (a) Gr/dop@Gr, (b) C_3N/dop@Gr, (c) BC3/dop@Gr and (d) BN/dop@Gr HTSs within PBE functional. The zero of energy is at Fermi-level.

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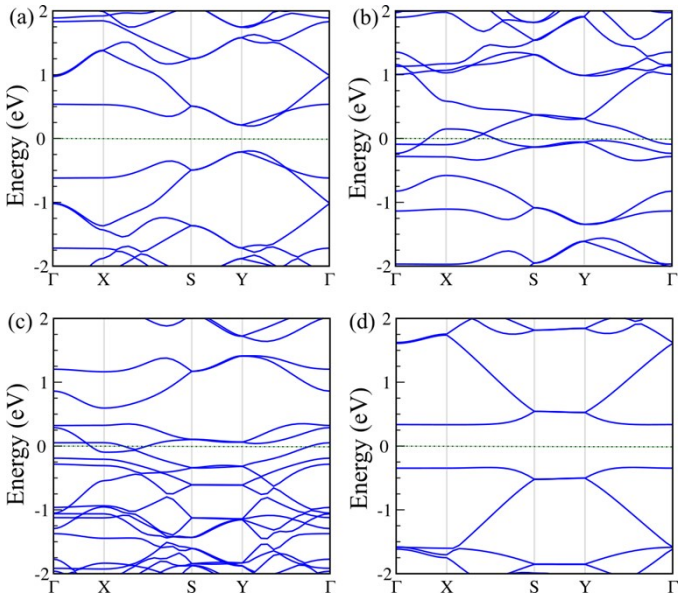

Fig. S5. The electronic band structure of (a) Gr-dop@Gr, (b) C_3N-dop@Gr, (c) BC3-dop@Gr and (d)BN-dop@Gr HTSs within PBE functional. The zero of energy is at Fermi-level.

*To whom correspondence should be addressed.
bafekry.asad@gmail.com