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

Supporting Information (SI)

Effects of different surface functionalization on the electronic properties and contact types of graphene/Functionalized-GeC van der Waals heterostructures

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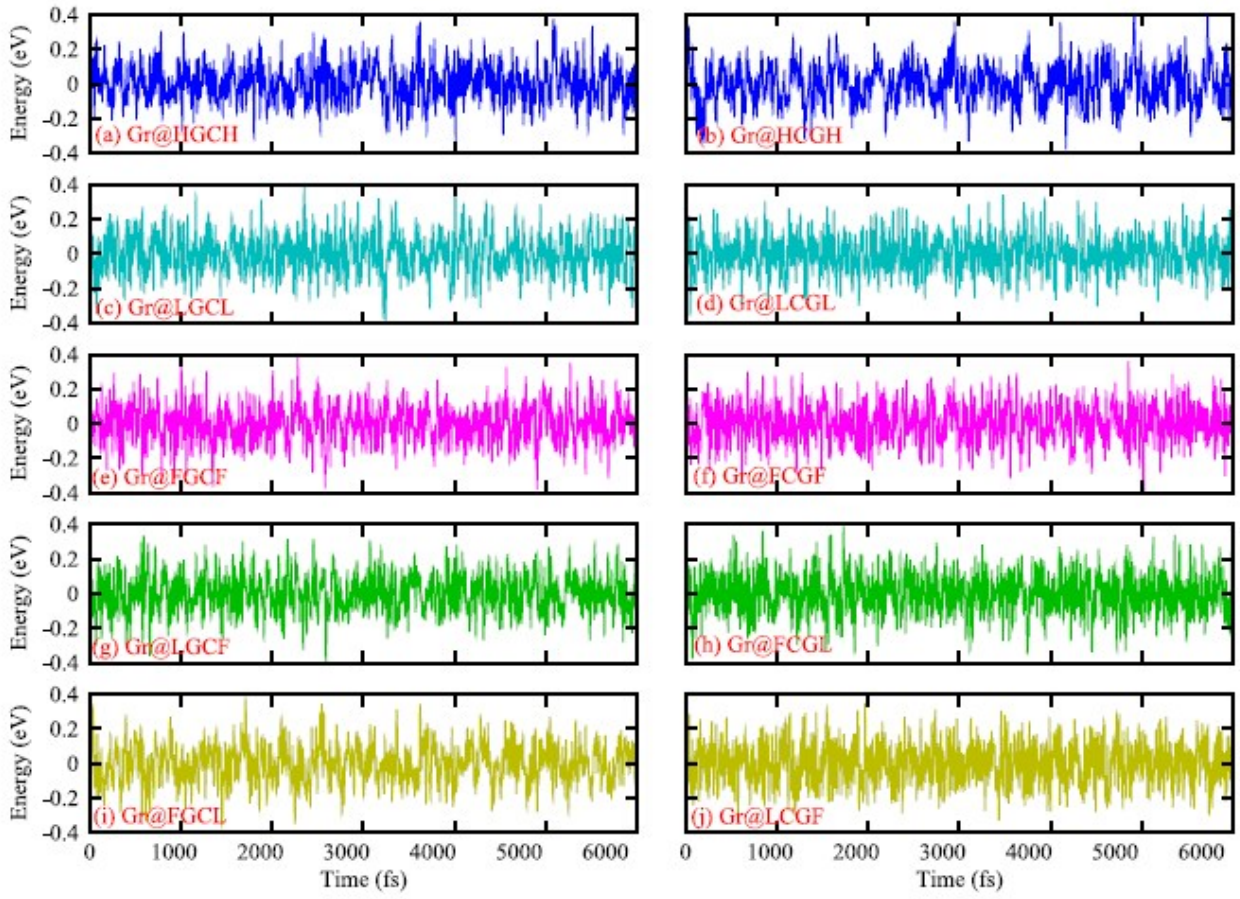

Fig. S1. AIMD simuations of the total energy fluctuation of all the Gr/Functionalized-GeC vdWHs at room temperature after 6 ps.

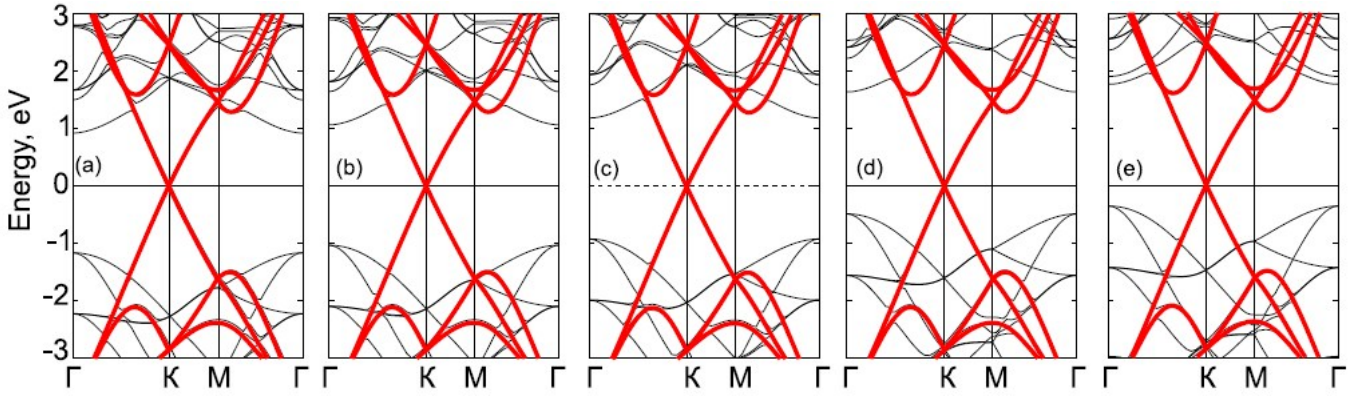

Fig. S2. Projected band structures of the Gr@LCGF heterostructure under different electric fields of (a) E = -0.2 V/Å, (b) E = -0.1 V/Å, (c) E = 0 V/Å, (d) E = +0.1 V/Å, (e) E = +0.2 V/Å. The Fermi level is set to be zero and marked by the dashed line.

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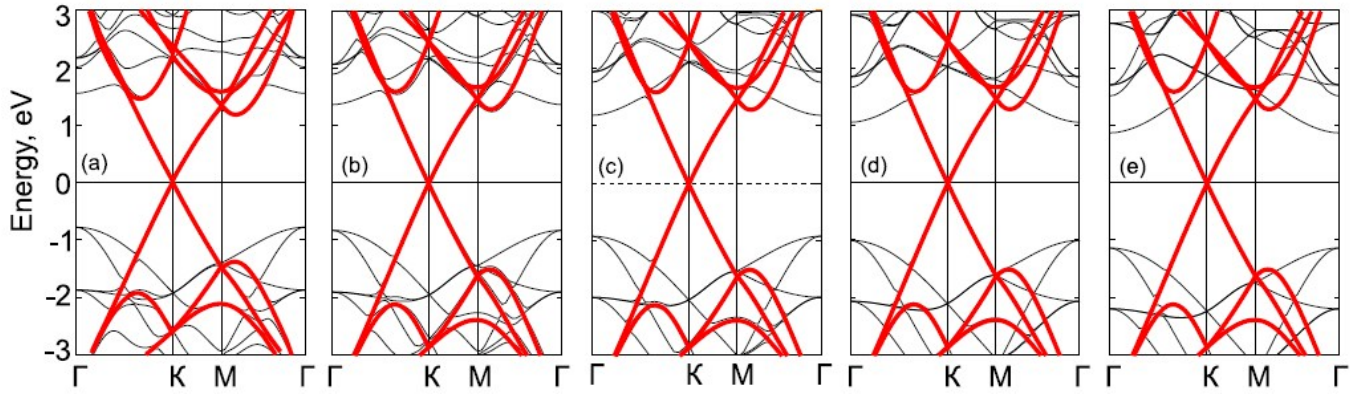

Fig. S3. Projected band structures of the Gr@LCGF heterostructure under different strains of (a) ΔD = -0.6 Å, (b) ΔD = -0.3 Å, (c) ΔD = 0 Å (unstrained), (d) ΔD = +0.3 Å, (e) ΔD = +0.6 Å. The Fermi level is set to be zero and marked by the dashed line.

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