Supporting Information

Exploring the effect of the covalent functionalization in graphene-antimonene heterostructures

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1. Computational studies

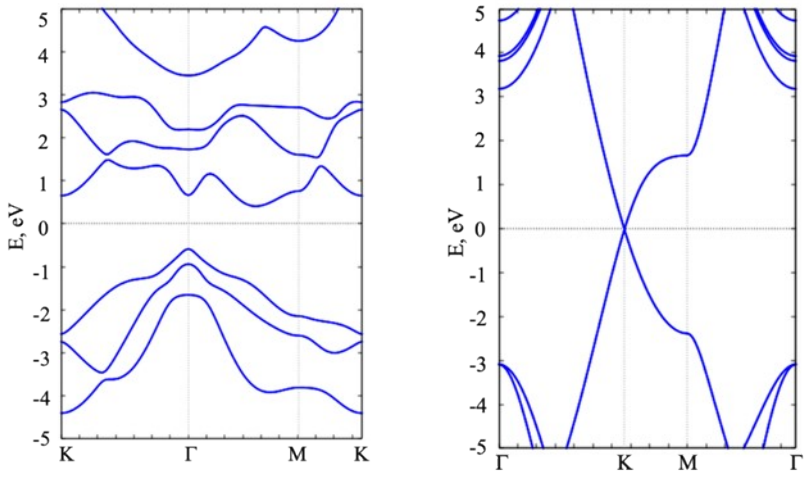

Figure S1: Band structure of (left) single layer Sb and (right) graphene including spin-orbit coupling (SOC) interaction.

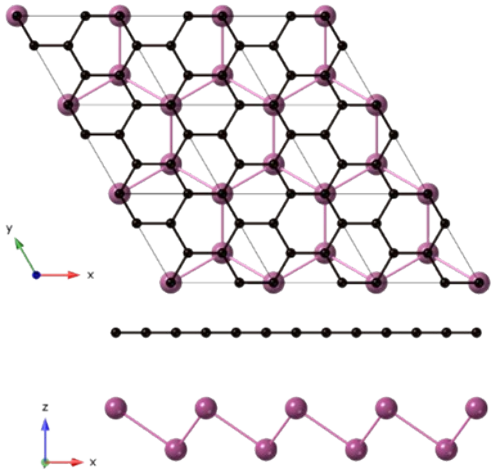

Figure S2: Top and lateral views of the heterostructure Sb/Graphene depicting a stacking where Sb atoms are placed below C atoms. Color code: C (black) and Sb (pink).

Table S1: Number of electrons transferred per cell via Bader charges analysis. Positive (negative) sign indicates gain (depletion) of electrons.

	Sb/Graphene
Sb	-0.0185
Graphene	0.0185

Table S2: Number of electrons transferred per cell via Bader charges analysis. Positive (negative) sign indicates gain (depletion) of electrons.

	Hybrid antimonene	Hybrid antimonene/graphene
Sb	-0.970	-0.978
C (tiol)	0.206	0.210
C (graphene)	-	0.006
S	1.003	1.006
H	-0.238	-0.245

2. Graphene functionalization at the Sb/graphene hybrid

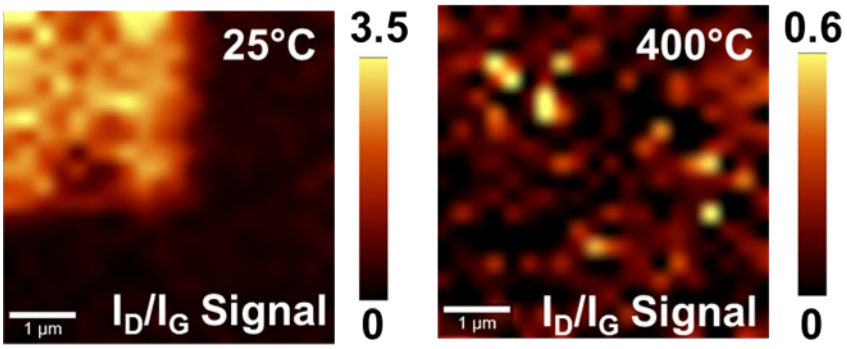

Figure S3: I_D/I_G ratio at room temperature (a) and at 400ºC (b) of the functionalized Sb NS/graphene hybrid area.