Supplementary material for manuscript:

The graphene/n-Ge(110) interface: structure, doping, and electronic properties

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Movie S1. The movie shows the binding energy scan through the valence band of the graphene/*n*-Ge(111) system for Sample A (two-graphene-domains sample). Left panel: Constant energy cuts at different binding energies; Brillouin zones with different K-points, K₁ and K₂, corresponding to two different graphene domains are marked by two dashed-line hexagons. Right panel: a series of the ARPES spectra along the $\Gamma - K_1$ direction (marked in the left panel) of the hexagonal graphene-derived Brillouin zone corresponding to one of the graphene domains; π_1 and π_2 states are marked in the plot. Data were collected with the PHOIBOS 100/2D-CCD analyzer and photon energy of $h\nu = 100 \text{ eV}$.

Movie S2. The movie shows the binding energy scan through the valence band of the graphene/*n*-Ge(111) system for Sample B (single-graphene-domain sample). Left panel: Constant energy cuts at different binding energies; Brillouin zone of graphene is marked by dashed-line hexagon. Right panel: a series of the ARPES spectra along the $K - \Gamma - K$ direction (marked in the left panel) of the hexagonal graphene-derived Brillouin zone. Data were collected with the KREIOS 150/2D-CCD analyzer and photon energy of $h\nu = 100 \text{ eV}$.

Table S3. A set of parameters obtained for different gr-Ge systems discussed in the text: graphene layer corrugation (in Å), mean distance between a graphene layer and top Ge layer (in Å), mean distance between layer of Sb dopants and top Ge layer for the intercalation-like systems (in Å), interaction energy (in meV per C-atom), position of the Dirac point with respect to the Fermi level (in meV). Considered systems: 1 - clean gr/Ge(110) interface (Fig. S4); 2 - gr/Ge(110) where 4 Sb atoms replace random Ge atoms in the top layer (Fig. S5); 3 - same as 2 but 4 Sb atoms replace Ge atoms in the 3rd Ge layer (Fig. S6); 4 - gr/Sb/Ge(110) intercalation-like system with concentration of 4 Sb atoms per (9 × 9) graphene supercell (Fig. S7); 5 - gr/Sb/Ge(110) intercalation-like system with concentration of 16 Sb atoms per (9 × 9) graphene supercell (Fig. S8); 6,7 - gr/Sb/Ge(110) intercalation-like system with concentration of 27 Sb atoms per (9 × 9) graphene supercell, before geometry optimization Sb atoms were placed either directly under C-atoms (6, Fig. S9) or in the center of the C-ring (7, Fig. S10).

	gr-corr.	gr-Ge dist.	Sb-Ge dist.	$E_{\rm int}$	$E_D - E_F$
System	(Å)	(Å)	(Å)	(meV/C-atom)	(meV)
1: gr/Ge(110)	0.09	3.54		-42	+195
2: $\operatorname{gr}/\operatorname{Ge}_x\operatorname{Sb}_y$	0.14	3.56		-42	+100
(4 Sb in layer 1)					
3: $\operatorname{gr}/\operatorname{Ge}_x\operatorname{Sb}_y$	0.09	3.52		-42	+165
(4 Sb in layer 3)					
4: gr/Sb/Ge	0.49	4.03	1.27	-32	+45
(4 Sb/u.c.)					
5: gr/Sb/Ge	0.42	4.91	1.47	-33	-95
$(16\mathrm{Sb/u.c.})$					
6: gr/Sb/Ge	0.43	5.50	2.03	-41	-170
$(27\mathrm{Sb/u.c.})$					
7: gr/Sb/Ge	0.43	5.46	1.96	-41	-125
$(27\mathrm{Sb/u.c.})$					



Figure S4. Top and side views of the clean gr/Ge(110) interface after geometry optimization (System 1, Table S3).



Figure S5. Top and side views of the gr/Ge(110) interface after geometry optimization where 4 Sb atoms replace random Ge atoms in the top layer (System 2, Table S3).



Figure S6. Top and side views of the gr/Ge(110) interface after geometry optimization where 4 Sb atoms replace random Ge atoms in 3rd layer (System 3, Table S3).



Figure S7. Top and side views of the gr/Sb/Ge(110) intercalation-like system after geometry optimization with concentration of 4 Sb atoms per (9×9) graphene supercell (System 4, Table S3).



Figure S8. Top and side views of the gr/Sb/Ge(110) intercalation-like system after geometry optimization with concentration of 16 Sb atoms per (9×9) graphene supercell (System 5, Table S3).



Figure S9. Top and side views of the gr/Sb/Ge(110) intercalation-like system after geometry optimization with concentration of 27 Sb atoms per (9×9) graphene supercell (System 6, Table S3). Before geometry optimization Sb atoms were placed directly under C-atoms.



Figure S10. Top and side views of the gr/Sb/Ge(110) intercalation-like system after geometry optimization with concentration of 27 Sb atoms per (9×9) graphene supercell (System 7, Table S3). Before geometry optimization Sb atoms were placed in the center of the C-rings.