Electronic Supplementary Material (ESI)

A new direct band gap Si-Ge allotrope with advanced electronic and optical properties

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Supporting Information

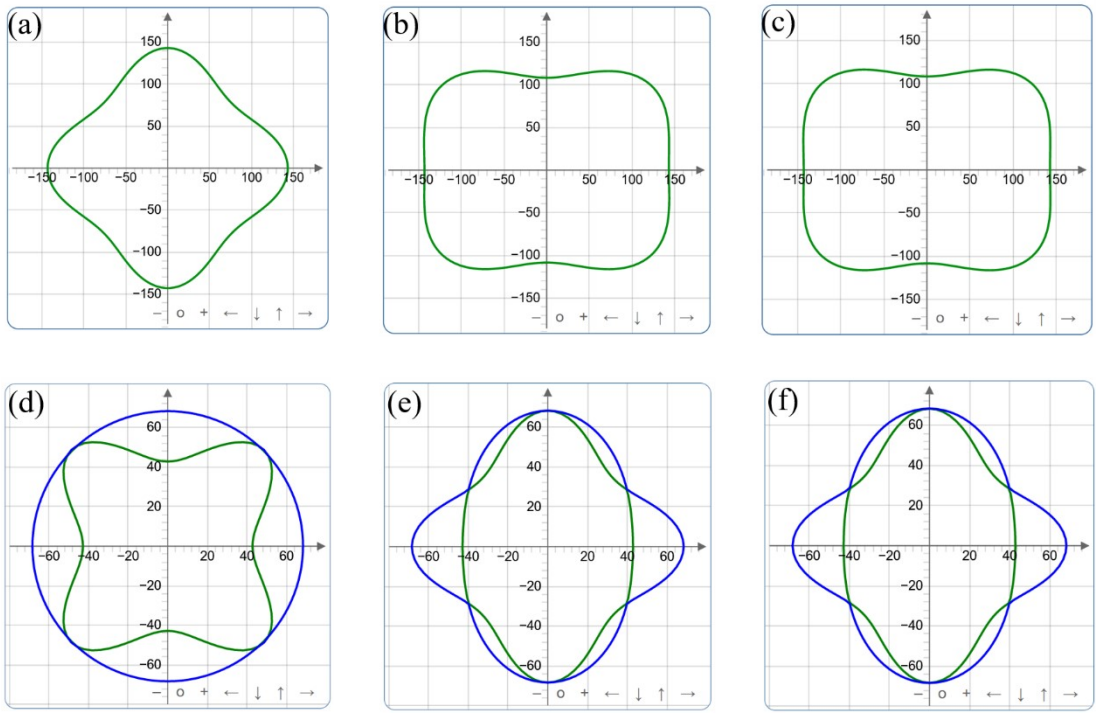

Figure S1 Spatial dependence of Young's modulus and shear modulus in α phase (in GPa). (a) Young's modulus in xy-plane, (b) xz-plane, and (c) yz-plane. (d) Shear modulus in xy-plane, (e) xz-plane, and (f) yz-plane.

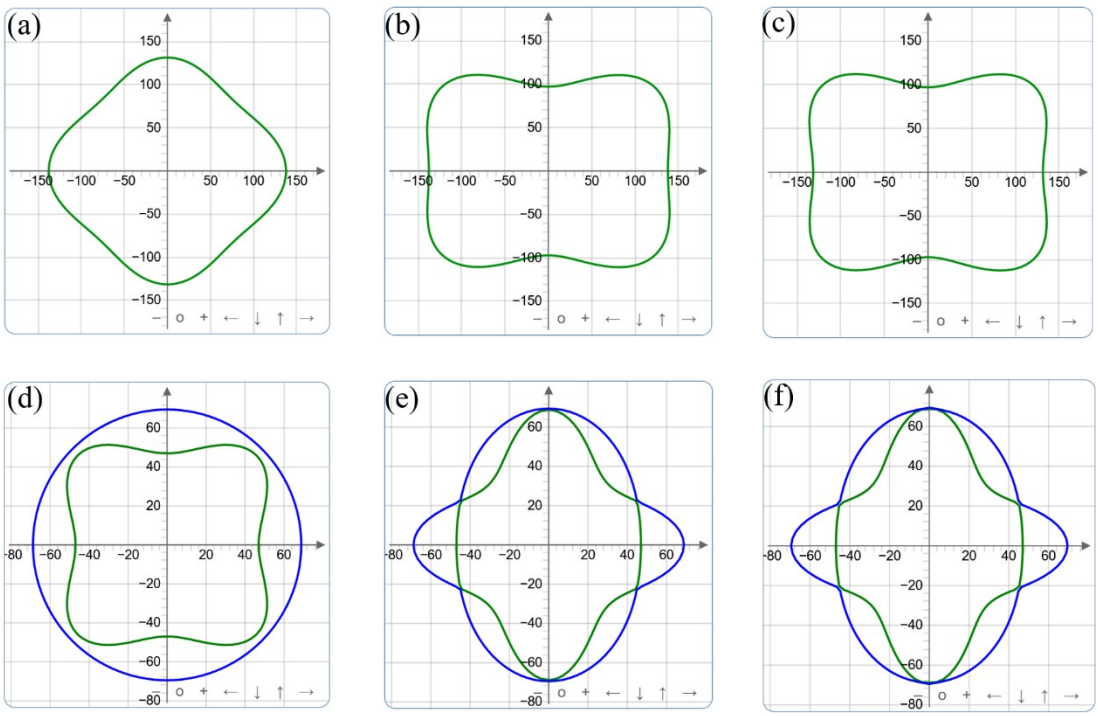

Figure S2 Spatial dependence of Young's modulus and shear modulus of β phase (in GPa). (a) Young's modulus in xy-plane, (b) xz-plane, and (c) yz-plane. (d) Shear modulus in xy-plane, (e) xz-plane, and (f) yz-plane.

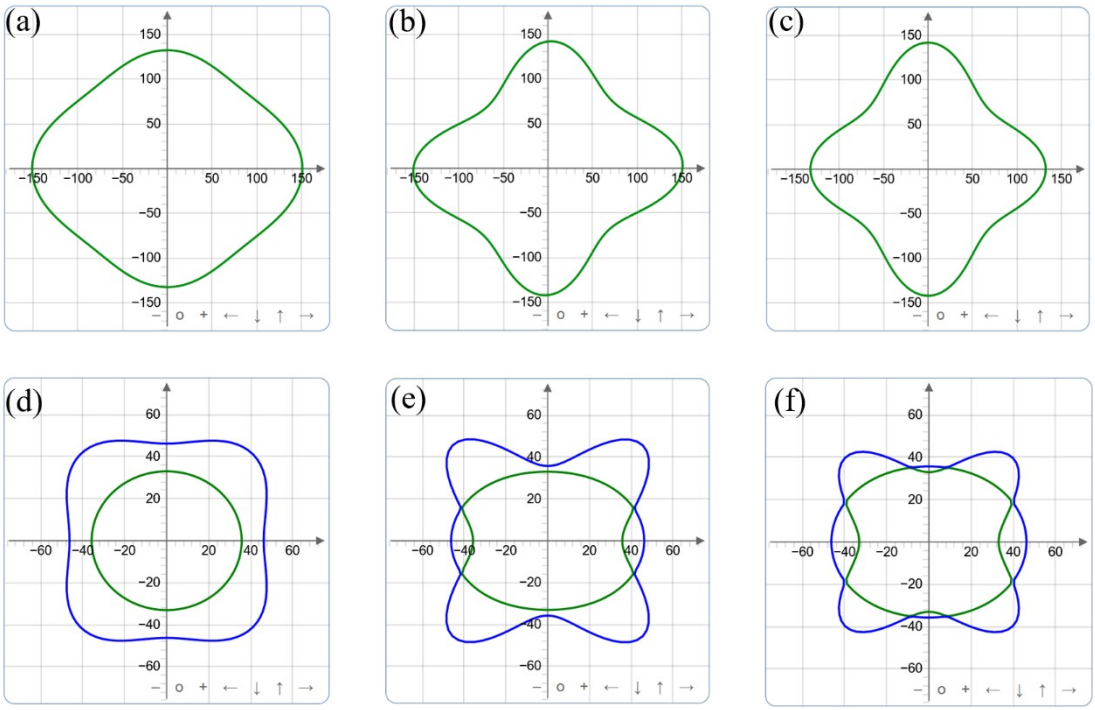

Figure S3 Spatial dependence of Young's modulus and shear modulus of γ phase (in GPa). (a) Young's modulus in xy-plane, (b) xz-plane, and (c) yz-plane. (d) Shear modulus in xy-plane, (e) xz-plane, and (f) yz-plane.

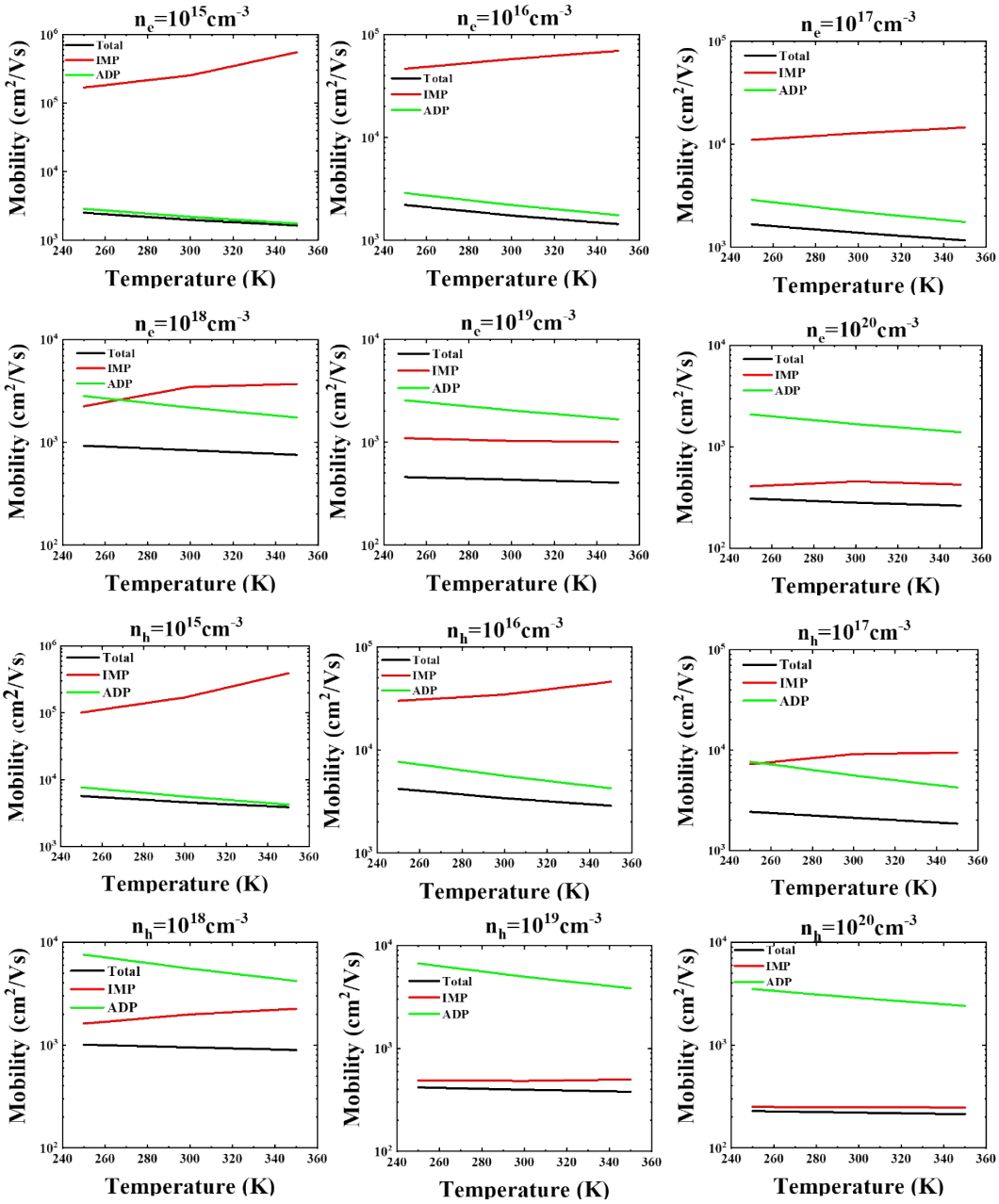

Figure S4 Calculated mobility of α phase under different temperatures and doping conditions, considering acoustic deformation potential (ADP) scattering (green line) and ionized impurity (IMP) scattering (red line). The black line represents the total carrier mobility.

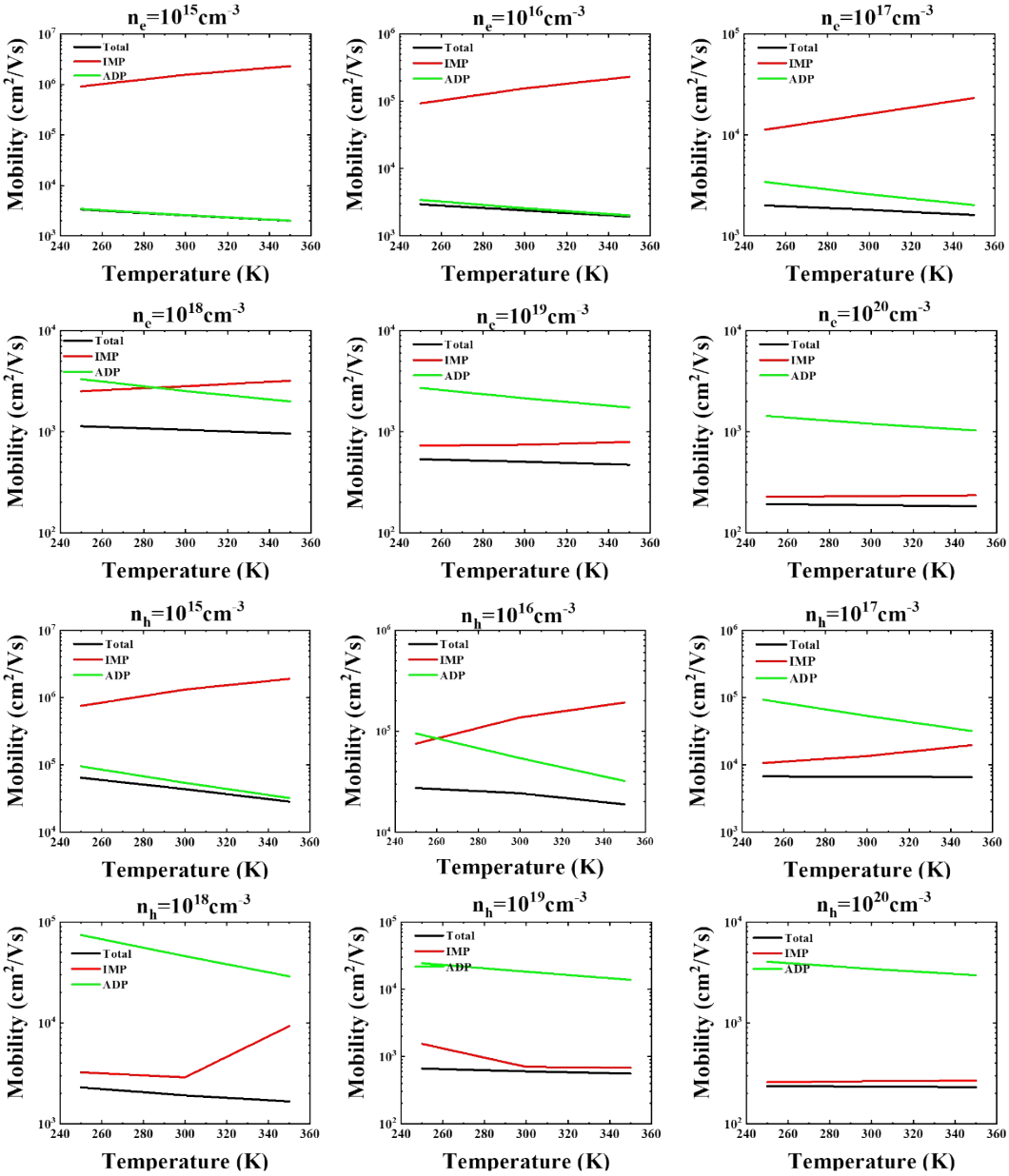

Figure S5 Carrier mobility of β phase under different temperatures and doping conditions, considering acoustic deformation potential (ADP) scattering (green line) and ionized impurity (IMP) scattering (red line). The black line represents the total carrier mobility.

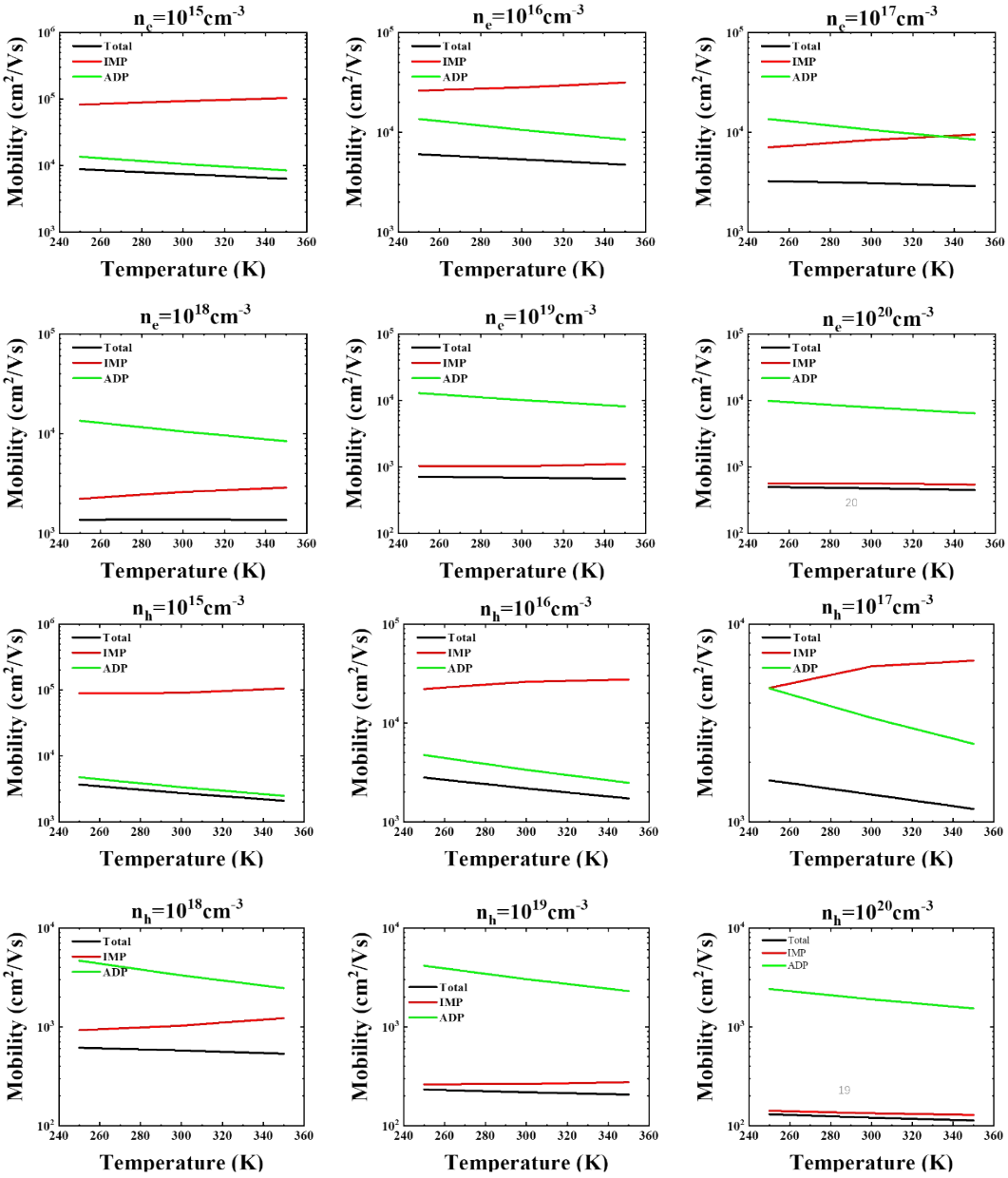

Figure S6 Carrier mobility of γ phase under different temperature and doping conditions, considering acoustic deformation potential (ADP) scattering (green line) and ionized impurity (IMP) scattering (red line). The black line represents the total carrier mobility.

Table S1 Selected structures and their basic properties found in this work

Chemical Formula	Space group No.	Total Energy (eV)	Band Gap (eV)	Character	Formation Energy (eV/atom)
Si_1Ge_4	1	-45.67	0.06	Indirect	0.13(5)
Si_2Ge_3	1	-48.48	0.28	Indirect	0.03(7)
	1	-47.94	0.80	Indirect	0.09(1)
	1	-47.86	0.85	Indirect	0.09(9)
	1	-47.78	0.21	Indirect	0.10(7)
	1	-47.75	0.18	Indirect	0.10(9)
Si_3Ge_2	8	-50.45	0.57	Indirect	0.02(2)
	160	-50.43	0.53	Indirect	0.02(4)
	8	-50.42	0.70	Indirect	0.02(5)
	44	-50.42	0.49	Direct	0.02(5)
	8	-50.41	0.63	Indirect	0.02(6)
	44	-50.36	0.17	Direct	0.03(1)
Si_4Ge_1	12	-51.76	0.54	Indirect	0.07(4)
	1	-51.63	0.95	Indirect	0.08(7)
	1	-51.59	0.79	Indirect	0.09(0)
	6	-51.56	0.64	Indirect	0.09(3)
	1	-51.51	0.94	Indirect	0.09(9)
	69	-102.86	0.77	Direct	0.10(6)