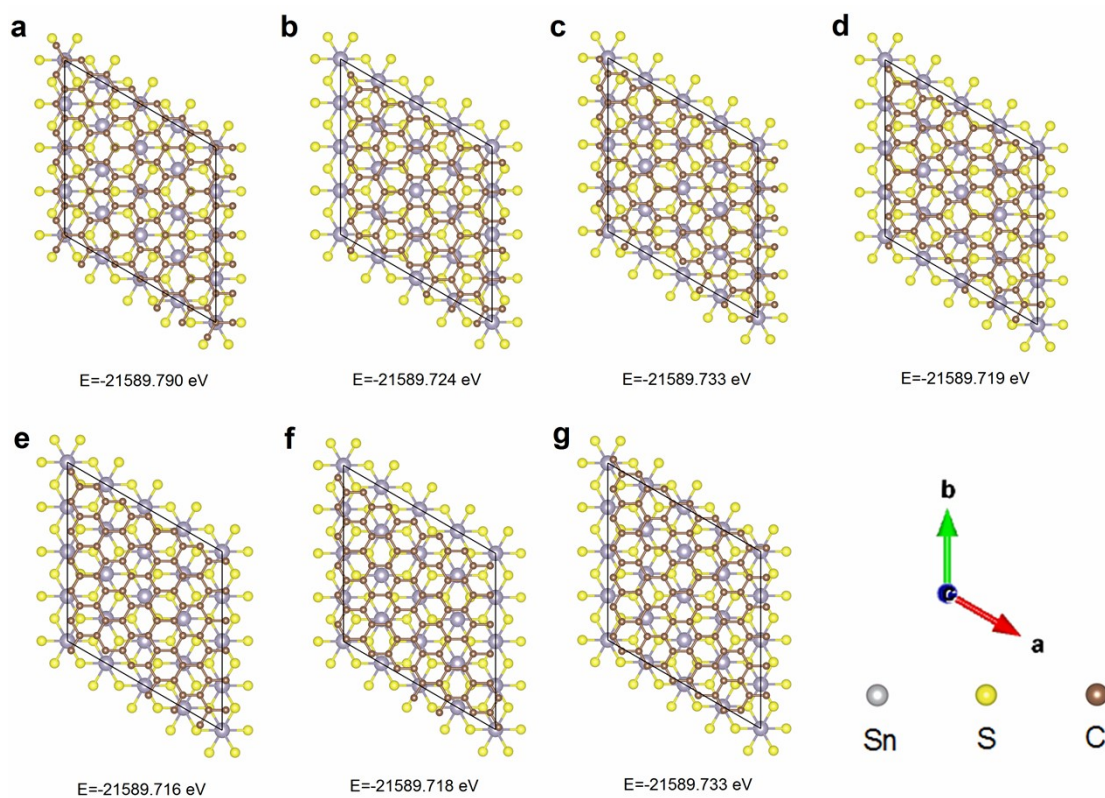
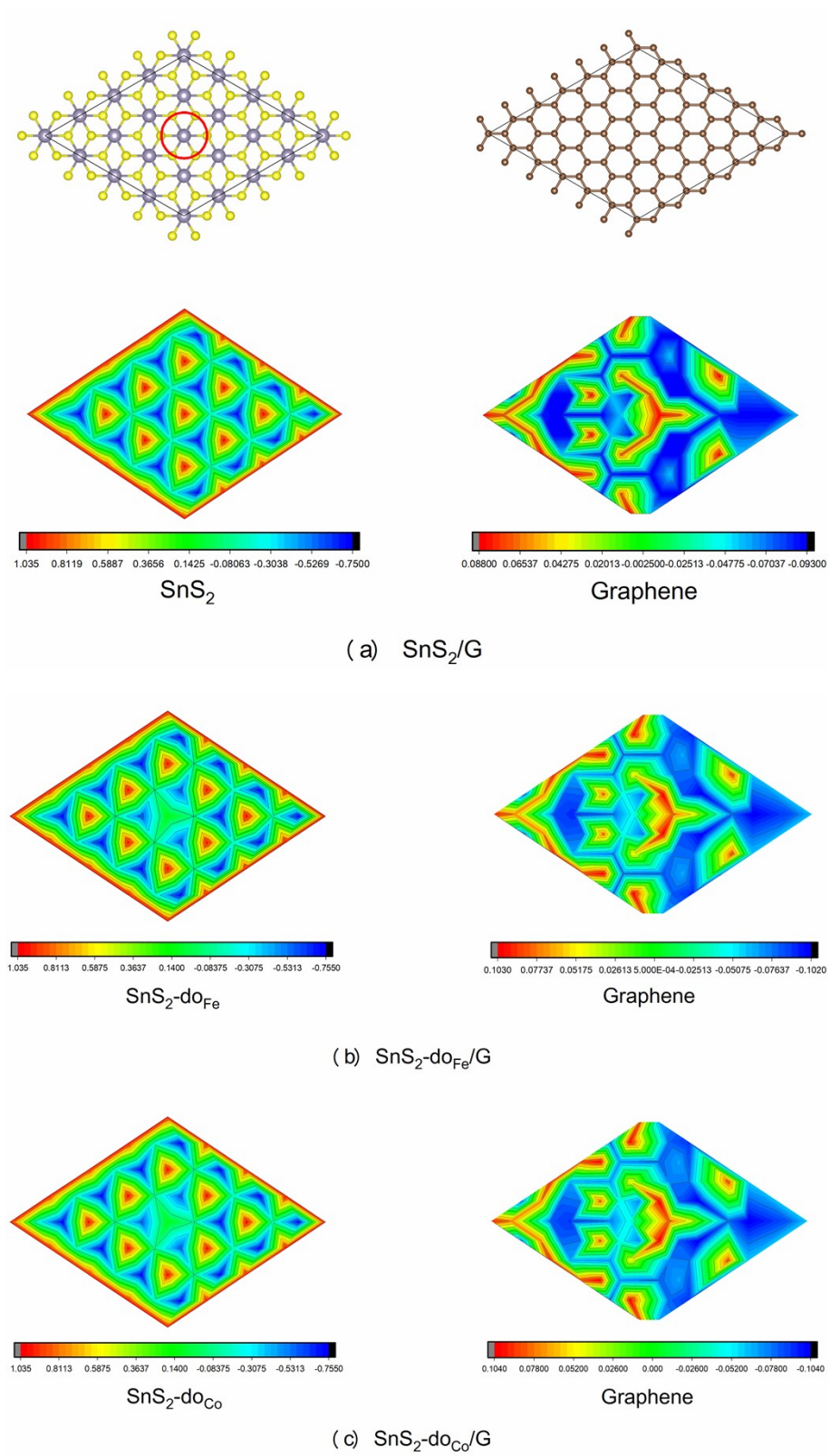


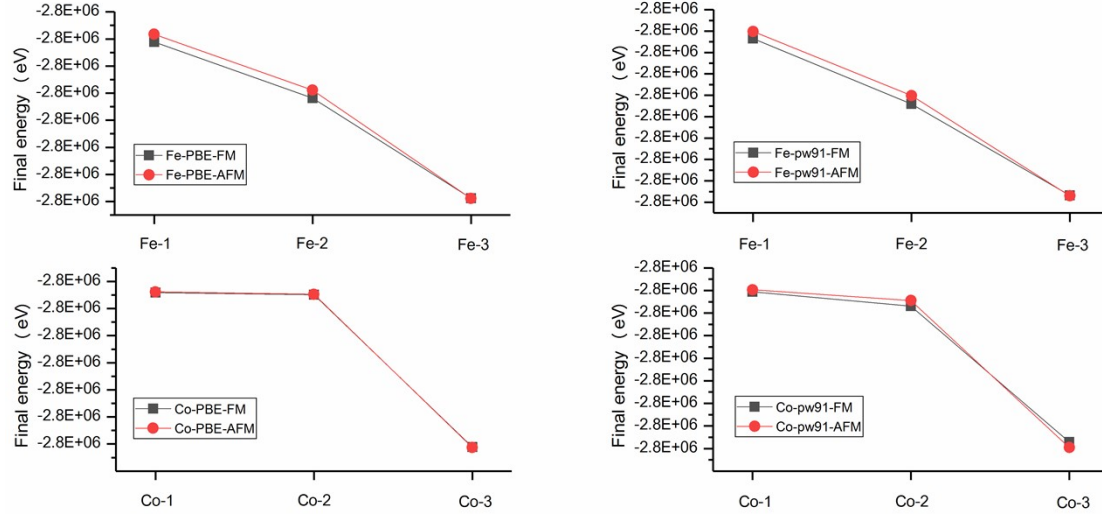
**Supplementary material**



**Fig. S1** Seven different initial relaxation positions of SnS<sub>2</sub>/G heterojunction system.



**Fig. S2** Charge distribution of intrinsic  $\text{SnS}_2/\text{G}$  and  $\text{Fe}^{3+}/\text{Co}^{3+}$  doped  $\text{SnS}_2/\text{G}$ . In the figure, the  $\text{SnS}_2$  and graphene counterparts are displayed separately.



**Fig. S3** Final energy of the three doping positions in Figure 9.

**Table S1** Mulliken atomic charge of  $\text{SnS}_2/\text{G}$ ,  $\text{SnS}_2\text{-do}_{\text{Fe}}/\text{G}$  and  $\text{SnS}_2\text{-do}_{\text{Co}}/\text{G}$ .

$\text{SnS}_2/\text{G}$		$\text{SnS}_2\text{-do}_{\text{Fe}}/\text{G}$		$\text{SnS}_2\text{-do}_{\text{Co}}/\text{G}$	
	charge		charge		charge
S(1)	-0.745	S(1)	-0.751	S(1)	-0.751
S(2)	-0.173	S(2)	-0.185	S(2)	-0.186
Sn(3)	1.025	Sn(3)	1.012	Sn(3)	1.011
S(4)	-0.745	S(4)	-0.751	S(4)	-0.751
S(5)	-0.121	S(5)	-0.086	S(5)	-0.081
Sn(6)	1.033	Sn(6)	1.016	Sn(6)	1.016
S(7)	-0.745	S(7)	-0.746	S(7)	-0.747
S(8)	-0.173	S(8)	-0.185	S(8)	-0.186
Sn(9)	1.025	Sn(9)	1.012	Sn(9)	1.011
S(10)	-0.745	S(10)	-0.746	S(10)	-0.747
S(11)	-0.121	S(11)	-0.123	S(11)	-0.124
Sn(12)	1.033	Sn(12)	1.033	Sn(12)	1.034
S(13)	-0.746	S(13)	-0.748	S(13)	-0.748
S(14)	-0.173	S(14)	-0.185	S(14)	-0.186
Sn(15)	1.033	Sn(15)	1.033	Sn(15)	1.034
S(16)	-0.745	S(16)	-0.593	S(16)	-0.586
S(17)	-0.173	S(17)	-0.083	S(17)	-0.093
Sn(18)	1.033	Sn(18)	1.017	Sn(18)	1.016
S(19)	-0.746	S(19)	-0.748	S(19)	-0.748
S(20)	-0.173	S(20)	-0.083	S(20)	-0.093
Sn(21)	1.033	Sn(21)	1.017	Sn(21)	1.016
S(22)	-0.745	S(22)	-0.746	S(22)	-0.747
S(23)	-0.173	S(23)	-0.185	S(23)	-0.186
Sn(24)	1.033	Sn(24)	1.033	Sn(24)	1.034
S(25)	-0.745	S(25)	-0.751	S(25)	-0.751
S(26)	-0.173	S(26)	-0.17	S(26)	-0.168

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Sn(27)	1.025	Sn(27)	1.012	Sn(27)	1.011
S(28)	-0.745	S(28)	-0.593	S(28)	-0.586
S(29)	-0.121	S(29)	-0.086	S(29)	-0.081
Sn(30)	1.033	Sn(30)	1.017	Sn(30)	1.016
S(31)	-0.745	S(31)	-0.593	S(31)	-0.586
S(32)	-0.173	S(32)	-0.083	S(32)	-0.093
Sn(33)	1.025	Fe(33)	0.13	Co(33)	0.119
S(34)	-0.745	S(34)	-0.751	S(34)	-0.751
S(35)	-0.121	S(35)	-0.086	S(35)	-0.081
Sn(36)	1.033	Sn(36)	1.017	Sn(36)	1.016
S(37)	-0.746	S(37)	-0.746	S(37)	-0.745
S(38)	-0.173	S(38)	-0.17	S(38)	-0.168
Sn(39)	1.033	Sn(39)	1.016	Sn(39)	1.016
S(40)	-0.745	S(40)	-0.751	S(40)	-0.751
S(41)	-0.173	S(41)	-0.17	S(41)	-0.168
Sn(42)	1.033	Sn(42)	1.016	Sn(42)	1.016
S(43)	-0.746	S(43)	-0.748	S(43)	-0.748
S(44)	-0.173	S(44)	-0.185	S(44)	-0.186
Sn(45)	1.033	Sn(45)	1.017	Sn(45)	1.016
S(46)	-0.745	S(46)	-0.751	S(46)	-0.751
S(47)	-0.173	S(47)	-0.185	S(47)	-0.186
Sn(48)	1.033	Sn(48)	1.017	Sn(48)	1.016
C(49)	0.088	C(49)	0.088	C(49)	0.087
C(50)	-0.056	C(50)	-0.066	C(50)	-0.068
C(51)	-0.092	C(51)	-0.082	C(51)	-0.081
C(52)	-0.093	C(52)	-0.092	C(52)	-0.092
C(53)	-0.092	C(53)	-0.082	C(53)	-0.081
C(54)	-0.056	C(54)	-0.066	C(54)	-0.068
C(55)	0.088	C(55)	0.088	C(55)	0.087
C(56)	-0.056	C(56)	-0.06	C(56)	-0.06
C(57)	-0.092	C(57)	-0.084	C(57)	-0.084
C(58)	-0.093	C(58)	-0.102	C(58)	-0.104
C(59)	-0.092	C(59)	-0.084	C(59)	-0.084
C(60)	-0.056	C(60)	-0.06	C(60)	-0.06
C(61)	-0.087	C(61)	-0.08	C(61)	-0.08
C(62)	0.072	C(62)	0.103	C(62)	0.104
C(63)	-0.087	C(63)	-0.077	C(63)	-0.074
C(64)	-0.093	C(64)	-0.08	C(64)	-0.078
C(65)	-0.092	C(65)	-0.078	C(65)	-0.077
C(66)	-0.093	C(66)	-0.08	C(66)	-0.078
C(67)	-0.087	C(67)	-0.077	C(67)	-0.074
C(68)	0.072	C(68)	0.103	C(68)	0.104
C(69)	-0.087	C(69)	-0.08	C(69)	-0.08
C(70)	-0.093	C(70)	-0.102	C(70)	-0.104

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C(71)	-0.092	C(71)	-0.084	C(71)	-0.084
C(72)	-0.093	C(72)	-0.102	C(72)	-0.104
C(73)	0.088	C(73)	0.088	C(73)	0.087
C(74)	0.072	C(74)	0.103	C(74)	0.104
C(75)	-0.087	C(75)	-0.077	C(75)	-0.074
C(76)	0.072	C(76)	0.049	C(76)	0.046
C(77)	0.088	C(77)	0.082	C(77)	0.083
C(78)	-0.056	C(78)	-0.046	C(78)	-0.046
C(79)	0.088	C(79)	0.082	C(79)	0.083
C(80)	0.072	C(80)	0.049	C(80)	0.046
C(81)	-0.087	C(81)	-0.077	C(81)	-0.074
C(82)	0.072	C(82)	0.103	C(82)	0.104
C(83)	0.088	C(83)	0.088	C(83)	0.087
C(84)	-0.056	C(84)	-0.06	C(84)	-0.06
C(85)	0.088	C(85)	0.096	C(85)	0.096
C(86)	-0.056	C(86)	-0.066	C(86)	-0.068
C( 87)	-0.092	C(87)	-0.082	C(87)	-0.081
C(88)	-0.093	C(88)	-0.08	C(88)	-0.078
C(89)	-0.092	C(89)	-0.078	C(89)	-0.077
C(90)	-0.056	C(90)	-0.046	C(90)	-0.046
C(91)	0.088	C(91)	0.082	C(91)	0.083
C(92)	-0.056	C(92)	-0.046	C(92)	-0.046
C(93)	-0.092	C(93)	-0.078	C(93)	-0.077
C(94)	-0.093	C(94)	-0.08	C(94)	-0.078
C(95)	-0.092	C(95)	-0.082	C(95)	-0.081
C(96)	-0.056	C(96)	-0.066	C(96)	-0.068
C(97)	-0.087	C(97)	-0.085	C(97)	-0.085
C(98)	0.072	C(98)	0.076	C(98)	0.076
C(99)	-0.087	C(99)	-0.085	C(99)	-0.085
C(100)	-0.093	C(100)	-0.092	C(100)	-0.092
C(101)	-0.092	C(101)	-0.082	C(101)	-0.081
C(102)	-0.093	C(102)	-0.08	C(102)	-0.078
C(103)	-0.087	C(103)	-0.077	C(103)	-0.074
C(104)	0.072	C(104)	0.049	C(104)	0.046
C(105)	-0.087	C(105)	-0.077	C(105)	-0.074
C(106)	-0.093	C(106)	-0.08	C(106)	-0.078
C(107)	-0.092	C(107)	-0.082	C(107)	-0.081
C(108)	-0.093	C(108)	-0.092	C(108)	-0.092
C(109)	0.088	C(109)	0.096	C(109)	0.096
C(110)	0.072	C(110)	0.076	C(110)	0.076
C(111)	-0.087	C(111)	-0.085	C(111)	-0.085
C(112)	0.072	C(112)	0.076	C(112)	0.076
C(113)	0.088	C(113)	0.096	C(113)	0.096
C(114)	-0.056	C(114)	-0.066	C(114)	-0.068

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C(115)	0.088	C(115)	0.088	C(115)	0.087
C(116)	0.072	C(116)	0.103	C(116)	0.104
C(117)	-0.087	C(117)	-0.08	C(117)	-0.08
C(118)	0.072	C(118)	0.103	C(118)	0.104
C(119)	0.088	C(119)	0.088	C(119)	0.087
C(120)	-0.056	C(120)	-0.066	C(120)	-0.068

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