First-principles study on ferromagnetism in 4H-SiC codoped with Al and Mn

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Contents:

1. Spatial spin density distribution in the stable configuration (0, 2);

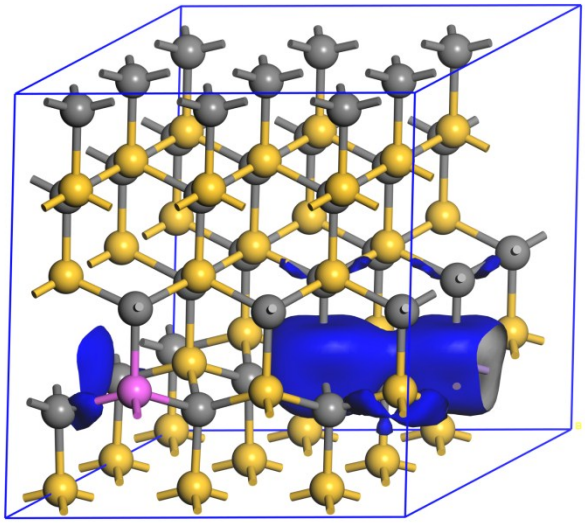

Fig. S1 (Color online) Spatial spin density distribution in the stable configuration (0, 2). The isosurface is 0.02 e/Å^3.

2. Schematic structure of 4H-SiC used to define (Al, 2Mn, V_{Si})-codoped 4H-SiC.

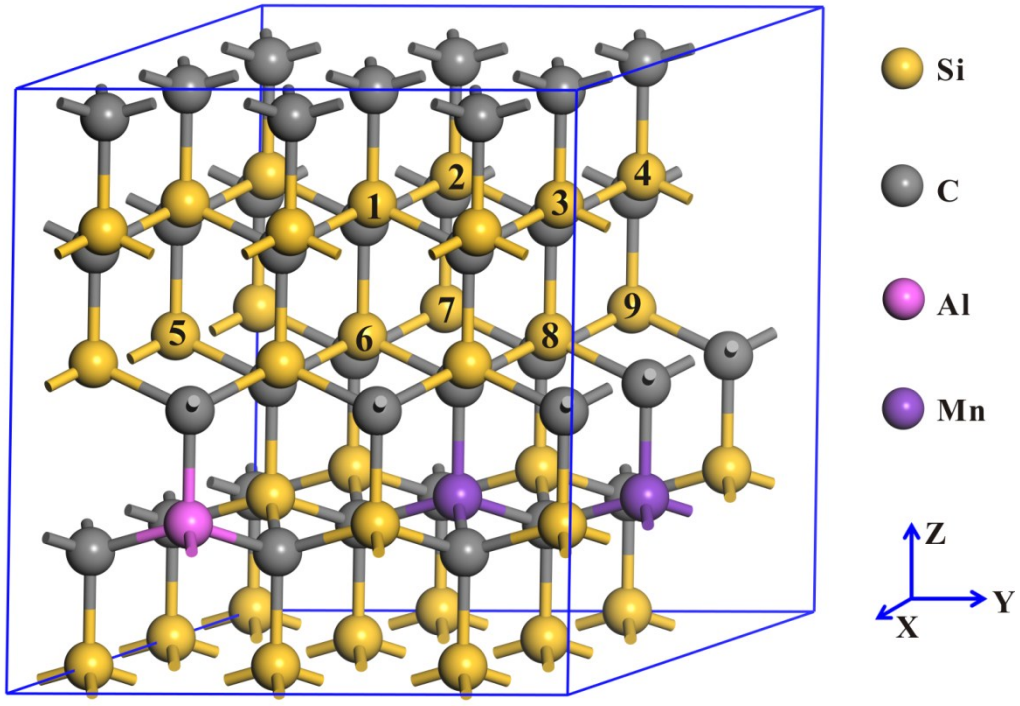

Fig. S2 (Color online) Schematic structure used to define (Al, 2Mn, V_{Si})-codoped 4H-SiC. Yellow, gray, pink, and purple spheres represent Si, C, Al and Mn atoms, respectively. Here, the positions of Si substituted by Al and the two Mn atoms are fixed while the positions substituted by V_{Si} are labelled by Arabic numerals varying from 1 to 9.

3. The calculated results of (Al, 2Mn, V_{Si})-codoped 4H-SiC.

Table S1. The optimized distance between Mn_1 and Mn_2 ($d_{Mn1\text{-}Mn2}$), the energy difference ΔE_d (meV) between FM and AFM states, the formation energies, E_f (eV) and the FM magnetic moments for Al (M_{Al}) and total magnetic moments for Mn (M_{Mn}) atoms are listed.

Configurations	$d_{Mn1\text{-}Mn2}$(Å)	ΔE_d (meV)	E_f(eV)	M_{Al} (μ_B)	M_{Mn} (μ_B, total)
1	3.078	45.0	13.01	0.00	5.12
2	3.078	-32.3	12.91	0.04	5.10
3	3.061	-68.9	13.03	0.02	5.02
4	3.083	-436.6	12.83	0.02	5.12
5	3.036	40.5	12.31	0.02	4.72
6	3.049	-105.9	12.36	0.02	4.24
7	3.063	-161.3	13.10	0.04	5.16
8	3.058	-65.6	11.90	0.02	4.28
9	3.069	-957.0	13.00	0.02	4.94

Note: $\Delta E_d = E_{FM} - E_{AFM}$