Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supporting Information

$FeSi_2$: a two-dimensional ferromagnet containing planar hexacoordinate Fe atoms

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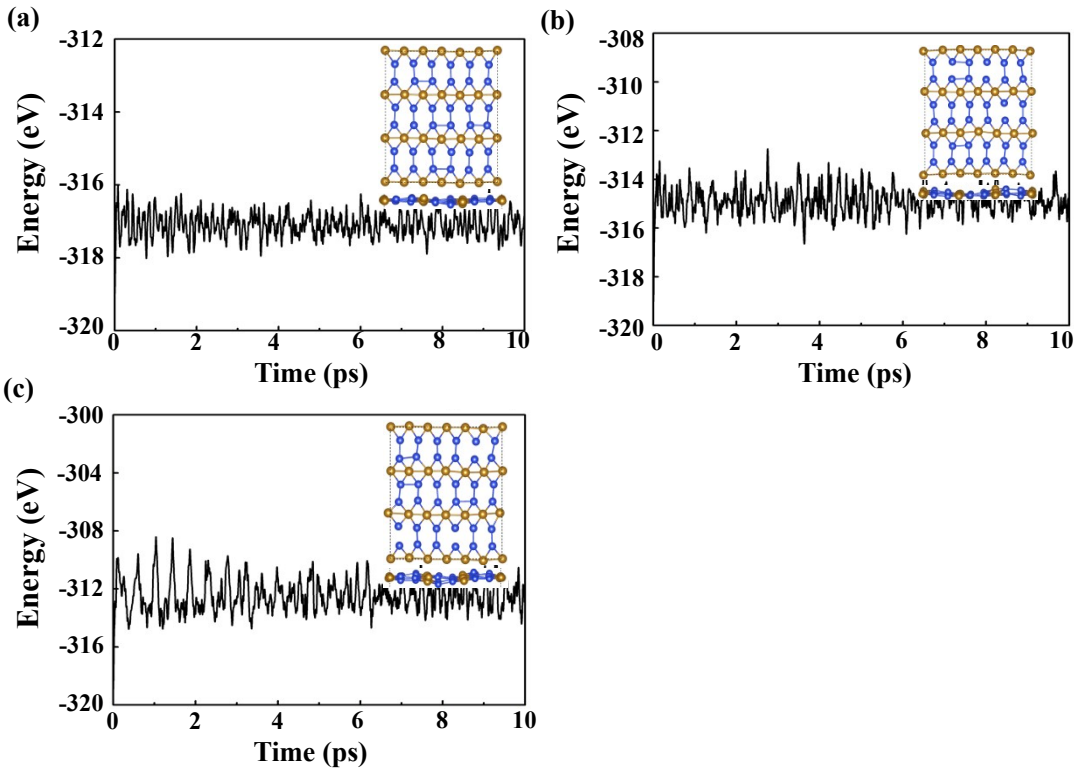

Fig. S1 Evolution of total energy for $FeSi_2$ monolayer at (a) 300 K, (b) 600 K, and (c) 900 K based on AIMD simulations. The insets show snapshots of the $FeSi_2$ monolayer equilibrium structure at different temperatures at the end of the 10-ps AIMD simulation.

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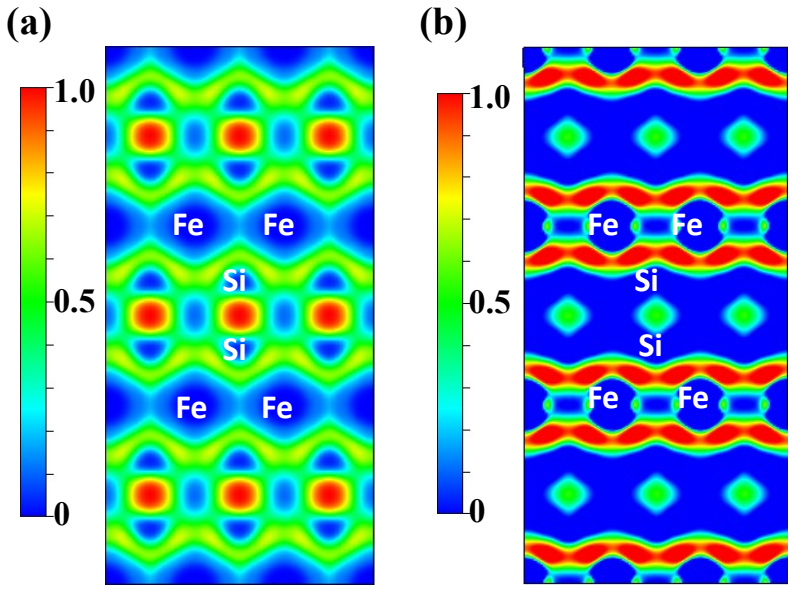

Fig. S2 (a) ELF maps corresponding to slices of $FeSi_2$ monolayer perpendicular to the (001) direction with an isosurface of 0.84 au. (b) Differential charge density slices of $FeSi_2$ monolayer perpendicular to the (001) direction with an isosurface of 0.008 e·Å^{-3}. Blue and red colors represent charge accumulation and depletion, respectively.

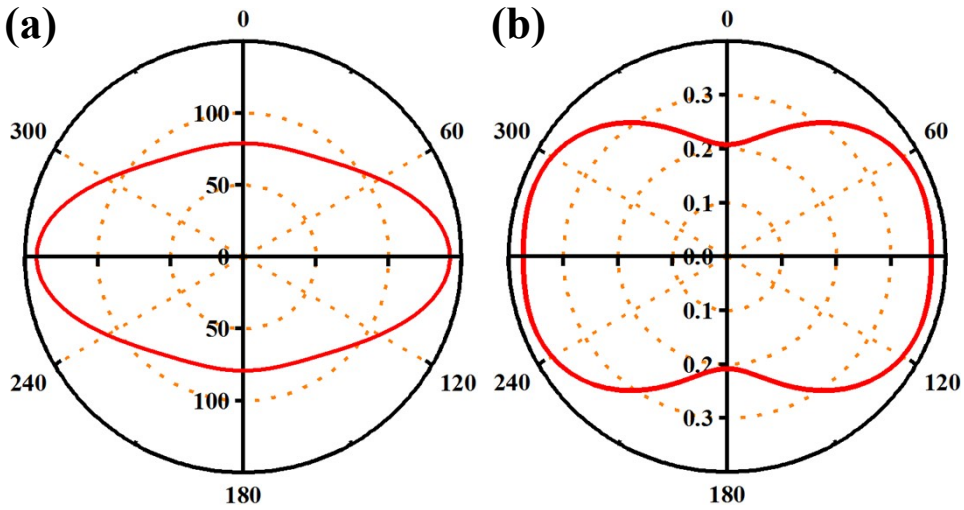

Fig. S3 Polar diagrams of the (a) Young's modulus and (b) Poisson's ratio of $FeSi_2$ monolayer.

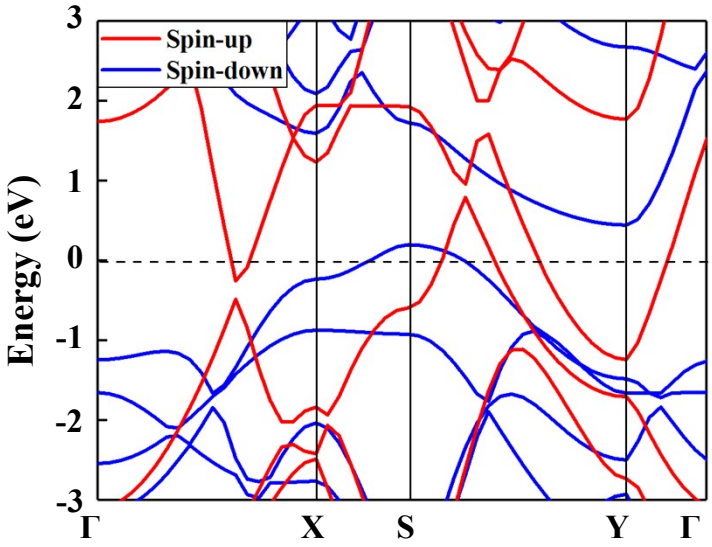

Fig. S4 Spin-polarized band structures of $FeSi_2$ monolayer calculated using the HSE06 functional.

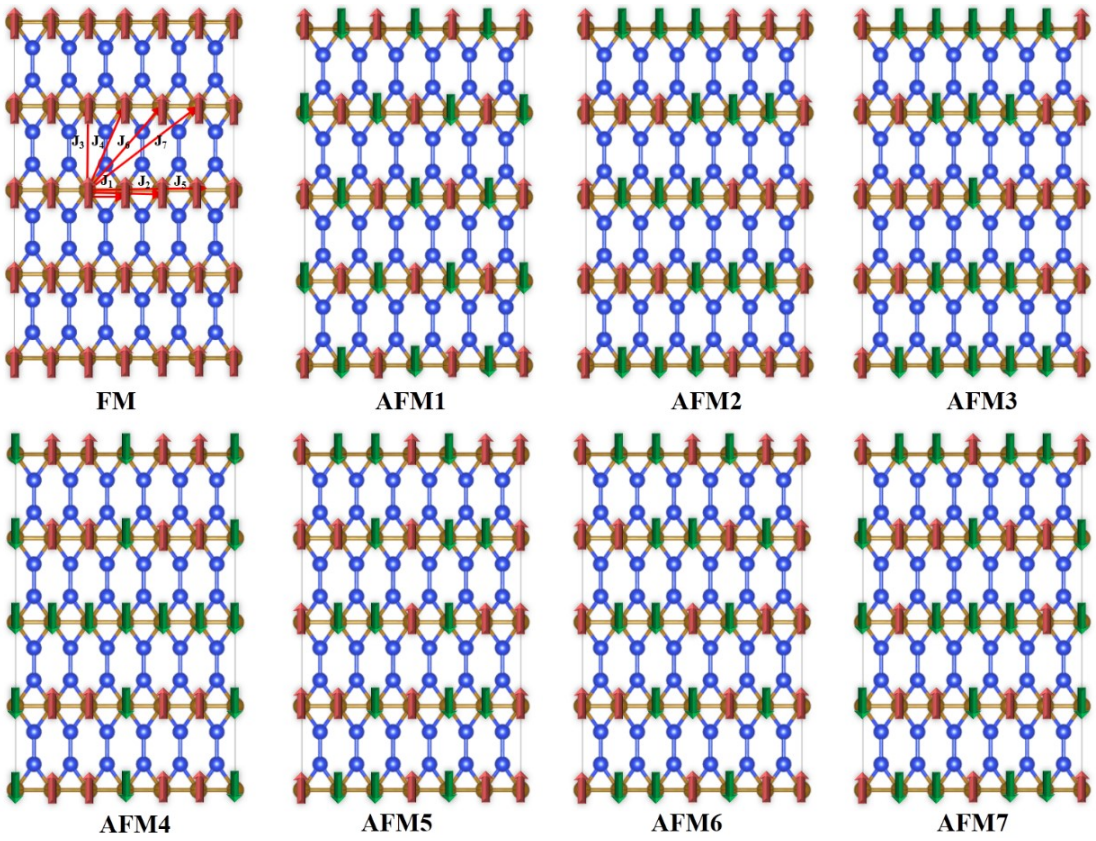

Fig. S5 Ferromagnetic (FM) state and seven different antiferromagnetic (AFM) states. Red and green indicate spin up and spin down, respectively. The exchange parameters of J_i (i = 1–7) are marked in the FM state.

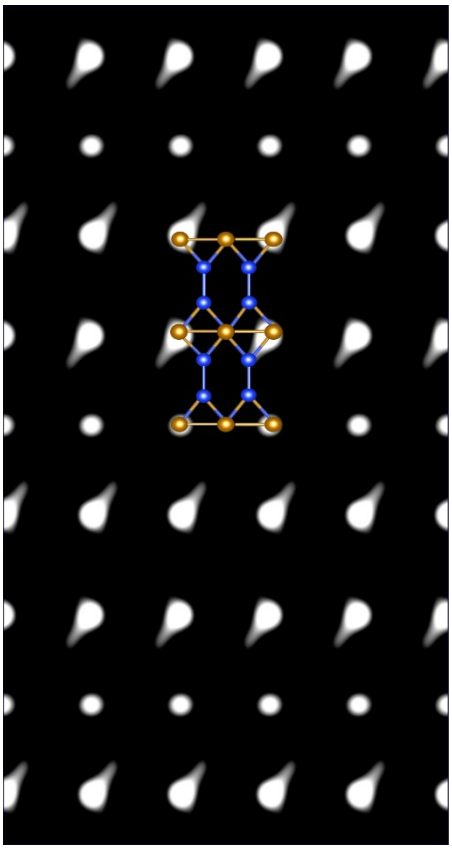

Fig. S6 Simulated constant-current STM images of $FeSi_2$ monolayer at a bias voltage of −1.32 eV at 2 Å above the Si (110) surface.

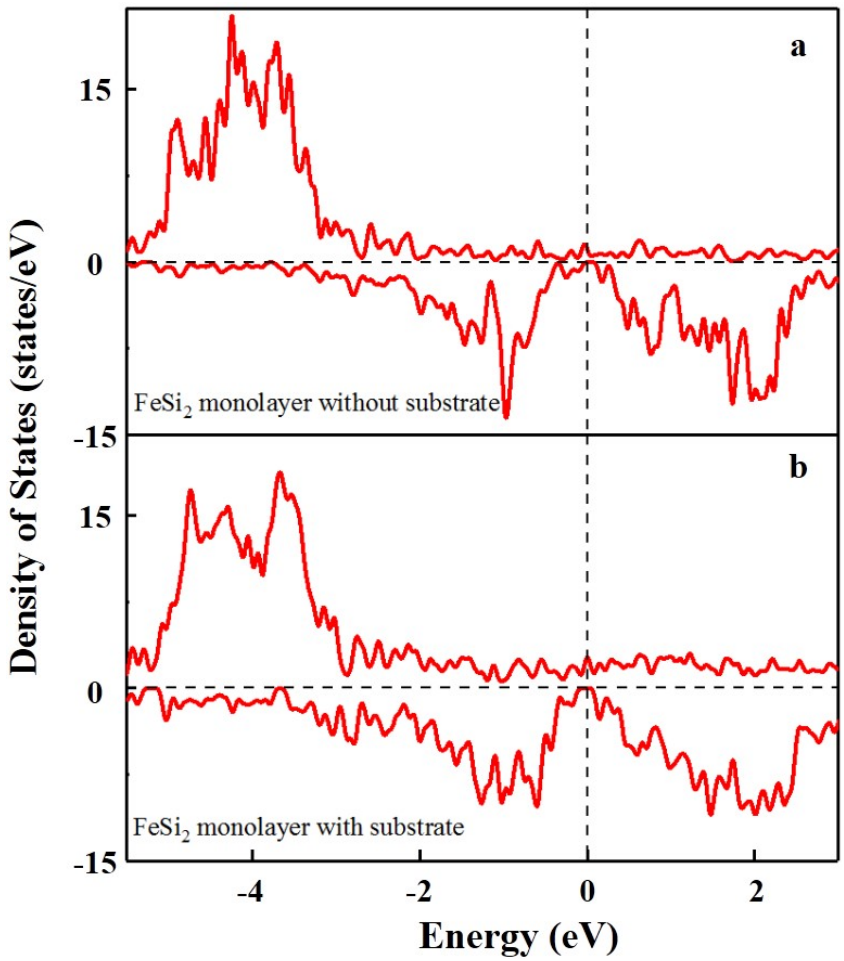

Fig. S7 DOS diagram of the freestanding $FeSi_2$ monolayer (a) with and (b) without the Si (110) substrate.

Table S1. The energy differences of different AFM states of $FeSi_2$ monolayer relative to the FM state in a 6×4×1 supercell, with unit is eV.

System	FM	AFM1	AFM2	AFM3	AFM4	AFM5	AFM6	AFM7
$FeSi_2$	0	2.09	1.72	0.86	1.43	1.70	1.75	2.10

Table S2. The calculated exchange parameters J_i (i = 1–7) of $FeSi_2$ monolayer at different distances d_i.

	$i = 1$	$i = 2$	$i = 3$	$i = 4$	$i = 5$	$i = 6$	$i = 7$
d_i (Å)	2.62	5.24	5.96	6.51	7.85	7.93	9.86
J_i (meV)	7.5	−4	2.3	3	0.85	−1.8	1.13