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RESEARCH ARTICLE

First-principles investigation of two-dimensional iron molybdenum nitride: A double transition-metal cousin of $MoSi_2N_4$(MoN) monolayer with distinctive electronic and topological properties

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Supporting Information

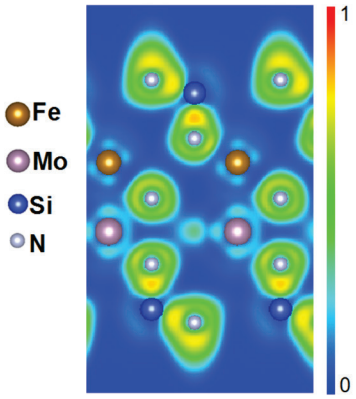

Fig. S1 The electron localization function (ELF) of $MoSi_2N_4$(FeN) monolayer, for which the atomic plane containing Fe-N, Mo-N, and Si-N bonds is chosen.

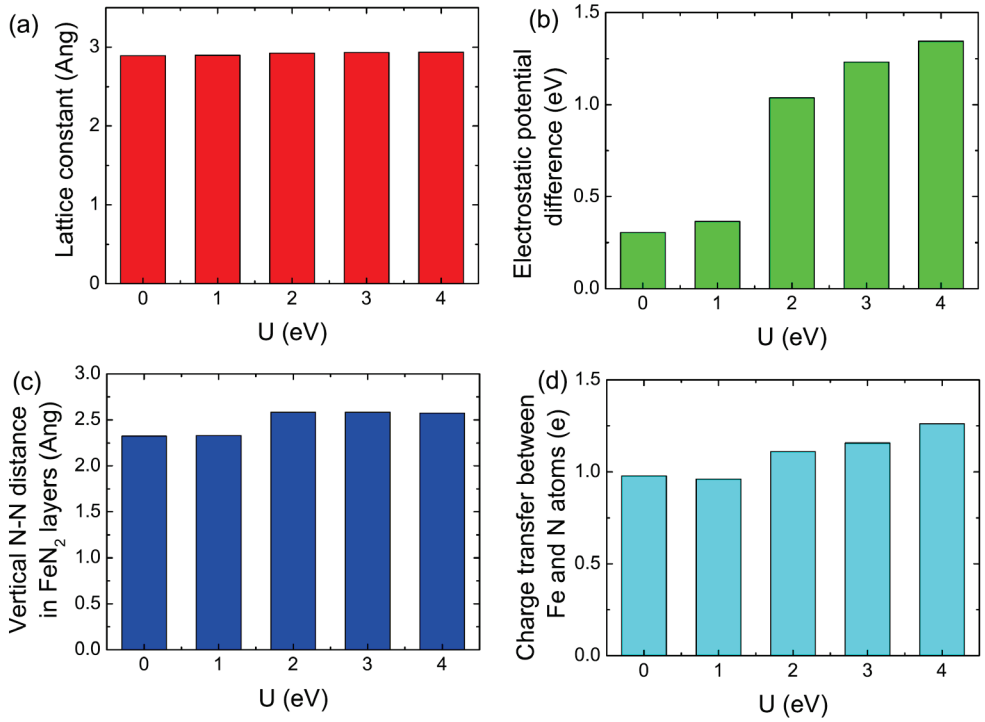

Fig. S2 The PBE+*U* results of $MoSi_2N_4$(FeN) monolayer. The variations of **(a)** lattice constant and **(b)** electrostatic potential difference of $MoSi_2N_4$(FeN) monolayer versus different *U* values in the PBE+*U* calculations. The corresponding variations of **(c)** the vertical N-N distance in the FeN_2 layer and **(d)** charge transfer between Fe and N atoms versus the *U* value.

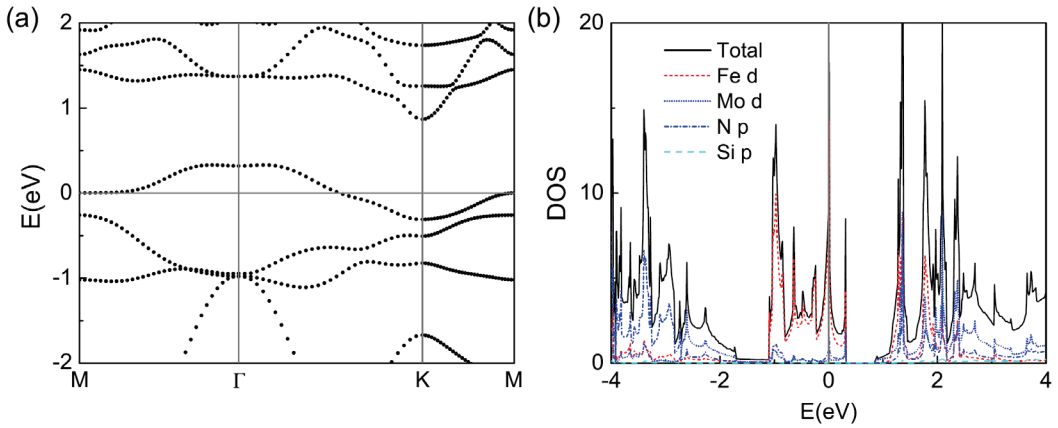

Fig. S3 The non-spin-polarized results of $MoSi_2N_4$(FeN) monolayer. **(a)** The band structures and **(b)** density of states of $MoSi_2N_4$(FeN) monolayer from the non-spin-polarized calculation.

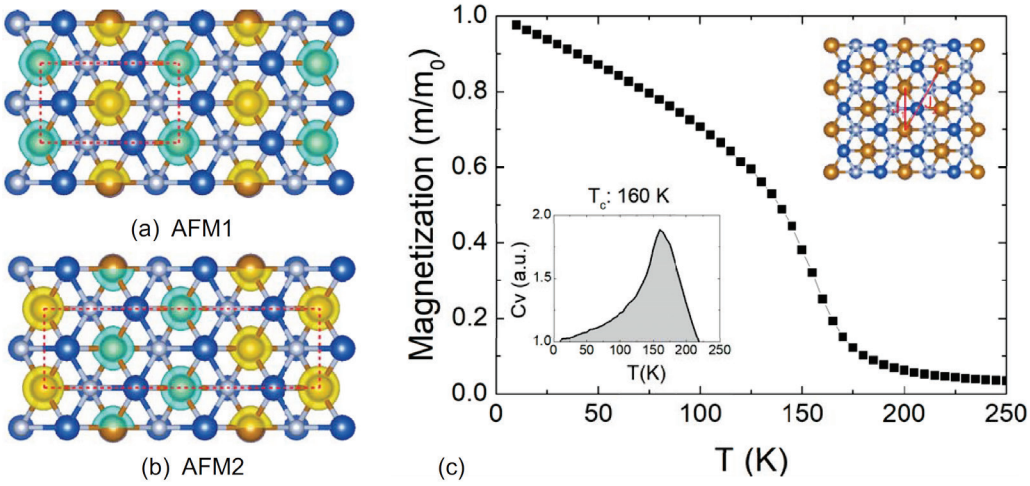

Fig. S4 The Monte Carlo simulation result of $MoSi_2N_4$(FeN) monolayer. The spin charge distribution of antiferromagnetic states in the **(a)** $1 \times \sqrt{3}$ and **(b)** $1 \times 2\sqrt{3}$ supercells for the $MoSi_2N_4$(FeN) monolayer. The isosurface is set to ±0.02 e/Å^3. **(c)** The Monte Carlo simulation on a Heisenberg model with the nearest (J_1) and next-nearest neighboring (J_2) exchange couplings. Through the energy mapping method, J_1 and J_2 are obtained as 9.9 and 1.8 meV, and the Curie temperature is estimated as 160 K.

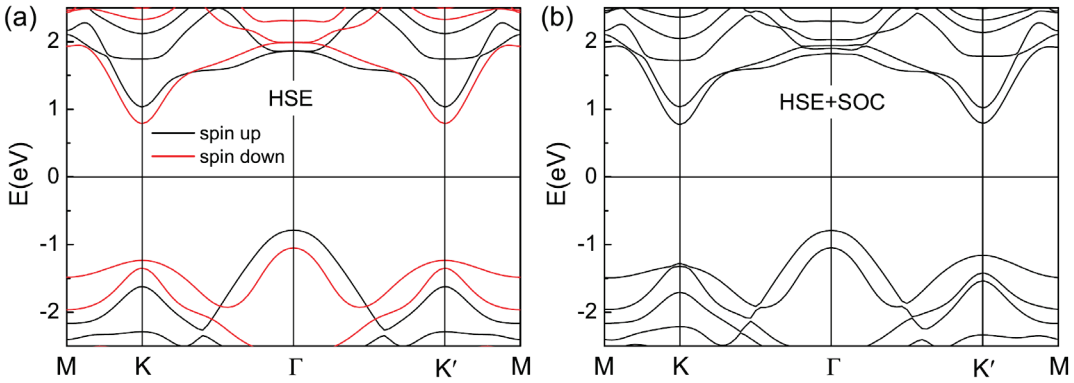

Fig. S5 The HSE and HSE+SOC bands of $MoSi_2N_4$(FeN) monolayer. A comparison of **(a)** HSE and **(b)** HSE+SOC band structures of the $MoSi_2N_4$(FeN) monolayer.

The POSCARs for $MoSi_2N_4$(FeN) and $MoSi_2N_4$(FeN)H monolayers.

1. $MoSi_2N_4$(FeN)

1.00000000000000

2.8907890178828830 0.0000000000000000 0.0000000000000000

-1.4453945089414415 2.5034967264676444 0.0000000000000000

0.0000000000000000 0.0000000000000000 25.8867546569545901

Mo N Si Fe

1 5 2 1

Direct

0.0000000000000000 0.0000000000000000 0.4526197735580632

0.3333333333333357 0.6666666666666643 0.5022449716157547

0.3333333333333357 0.6666666666666643 0.4040970537693799

0.6666666666666643 0.3333333333333357 0.5919582466445608

0.3333333333333357 0.6666666666666643 0.6797716907002416

0.6666666666666643 0.3333333333333357 0.3166285534273147

0.3333333333333357 0.6666666666666643 0.3365866691205788

0.6666666666666643 0.3333333333333357 0.6598737987703425

0.0000000000000000 0.0000000000000000 0.5562192423937633

2. $MoSi_2N_4$(FeN)H

1.00000000000000

2.8729689506860647 0.0000000000000000 0.0000000000000000

-1.4364844753430324 2.4880640955780535 0.0000000000000000

0.0000000000000000 0.0000000000000000 27.0180463391705636

Mo N Si Fe H

1 5 2 1 1

Direct

0.0000000000000000 0.0000000000000000 0.4284191476954482

0.3333333333333357 0.6666666666666643 0.4767195841426872

0.3333333333333357 0.6666666666666643 0.3818626480216861

0.3333333333333357 0.6666666666666643 0.5866501324188383

0.0000000000000000 0.0000000000000000 0.6591264767967846

0.6666666666666643 0.3333333333333357 0.2978511575580470

0.3333333333333357 0.6666666666666643 0.3172291801520648

0.6666666666666643 0.3333333333333357 0.6244031978619795

0.0000000000000000 0.0000000000000000 0.5307099326725301

0.0000000000000000 0.0000000000000000 0.6970285426799772