

Supporting Information of:

Magnetic monolayer of Elemental 2D Metals

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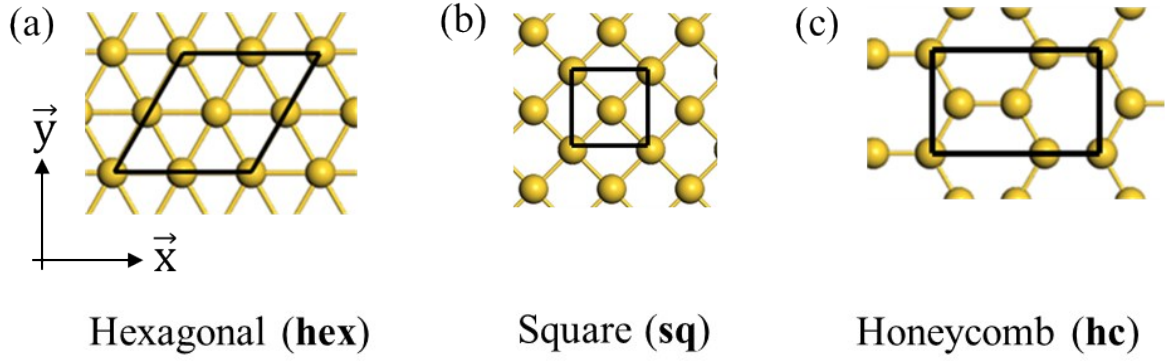


FIG. S1. The three 2D lattice structures. Yellow spheres denote metal atoms; black lines indicate the supercells constructed to consider different magnetic configurations. Note that a supercell is needed to consider the anti-ferromagnetic configurations.

Table S1. Some 2D metals and their structure types, for both theoretical and experimental works.

Elements	Structures	Experiment/Theory
Fe (in graphene nanopores)	sq	Experiment ¹
Mo (in monolayer MoSe ₂ nanopores)	hex	Experiment ²
Sn (on Cu(111))	hc	Experiment ³
Au (in bulk Au-Ag alloy nanopores)	hex	Experiment ⁴
Pb/In (on Si(111))	hex/sq	Experiment ⁵
Hf (on Ir(111))	hc	Experiment ⁶
Cr	hex, sq, hc	Experiment and Theory ⁷
Au	hc	Theory ⁸
Ag	hex, sq, hc	Theory ⁹

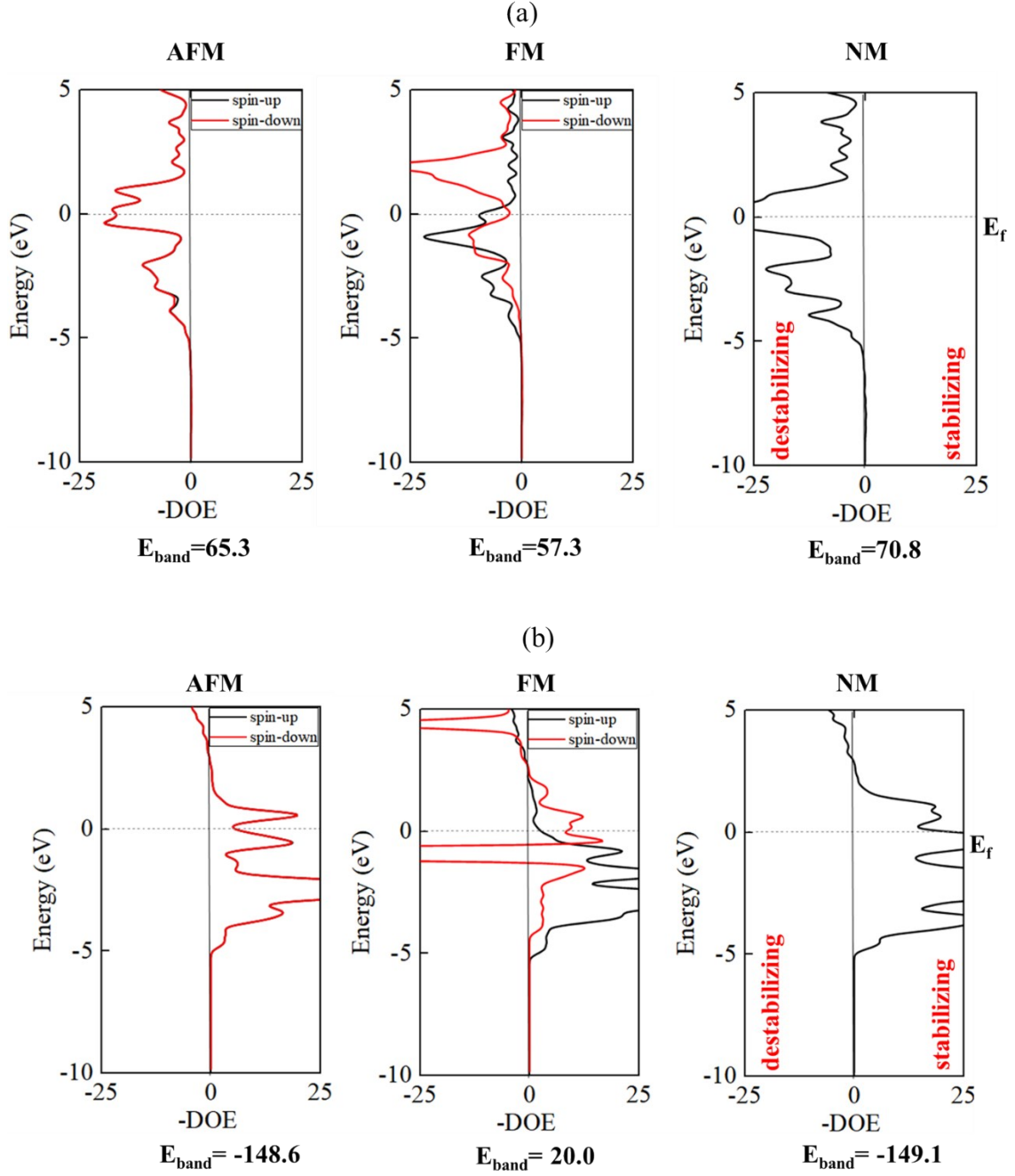


FIG. S2. DOE analysis of (a) bulk Fe and (b) hc Fe in three magnetic structures (nonmagnetic, FM, AFM). The fermi energy was set to zero (E_f). E_{band} represent the energy integral of the DOE in a energy range (Eq. 2 in the main text).

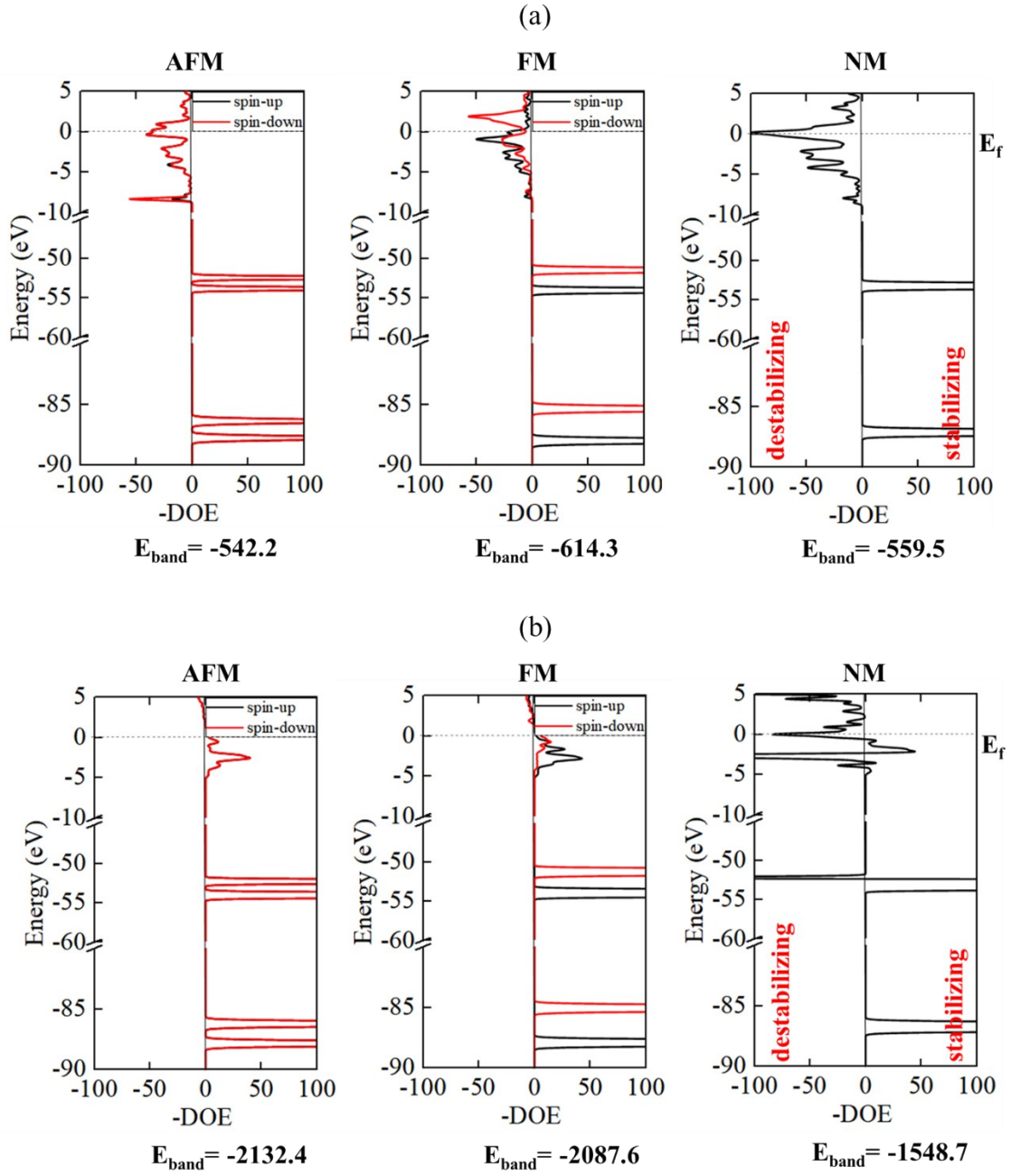


FIG. S3. Extended energy-range DOE analysis of (a) bulk Fe and (b) hc Fe in the three magnetic structures. The Fermi energy (E_F) was set to zero. E_{band} represent the energy integral of the DOE in a energy range including semi-core states.

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