Supplemental material

Strain modulated ferromagnetic phase transitions in monolayer $FeCl_2$ through exchange competitions: the first-principle and Monte Carlo simulations

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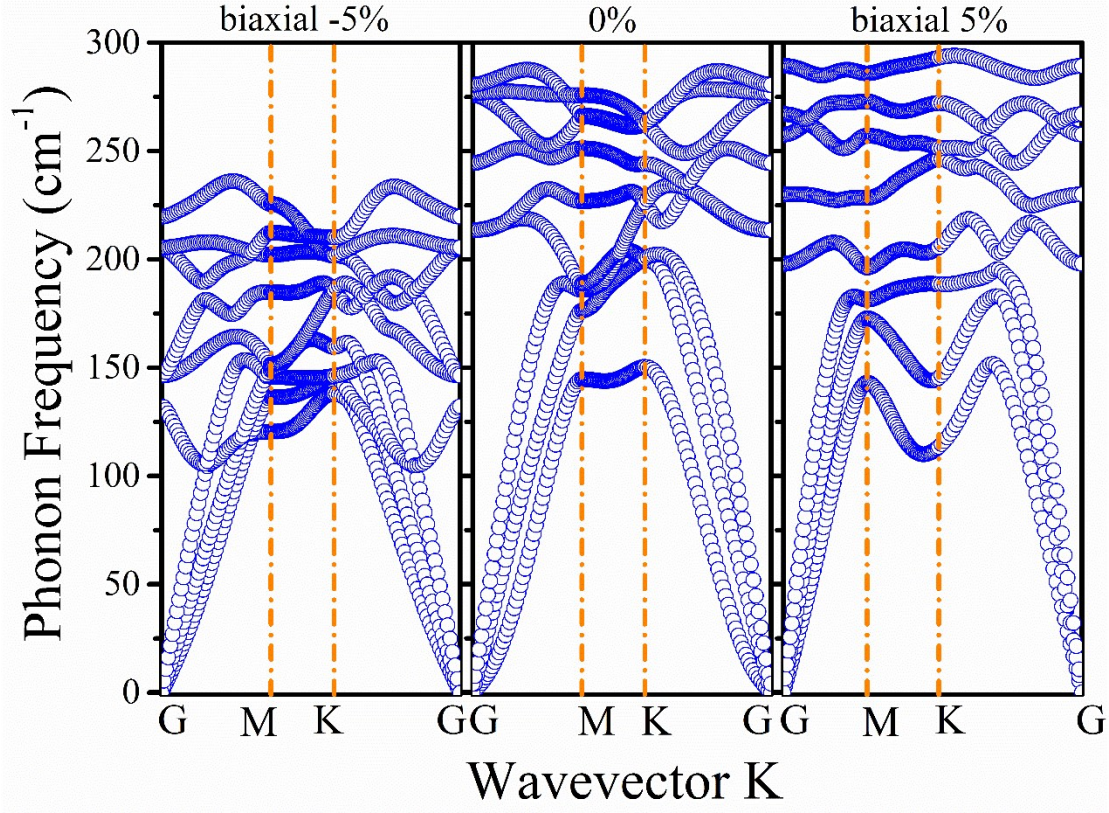

Fig.S1 The phonon dispersion of no-strain, biaxial ±5% monolayer $FeCl_2$. A triangle cell was adopted and no imaginary frequency appears.

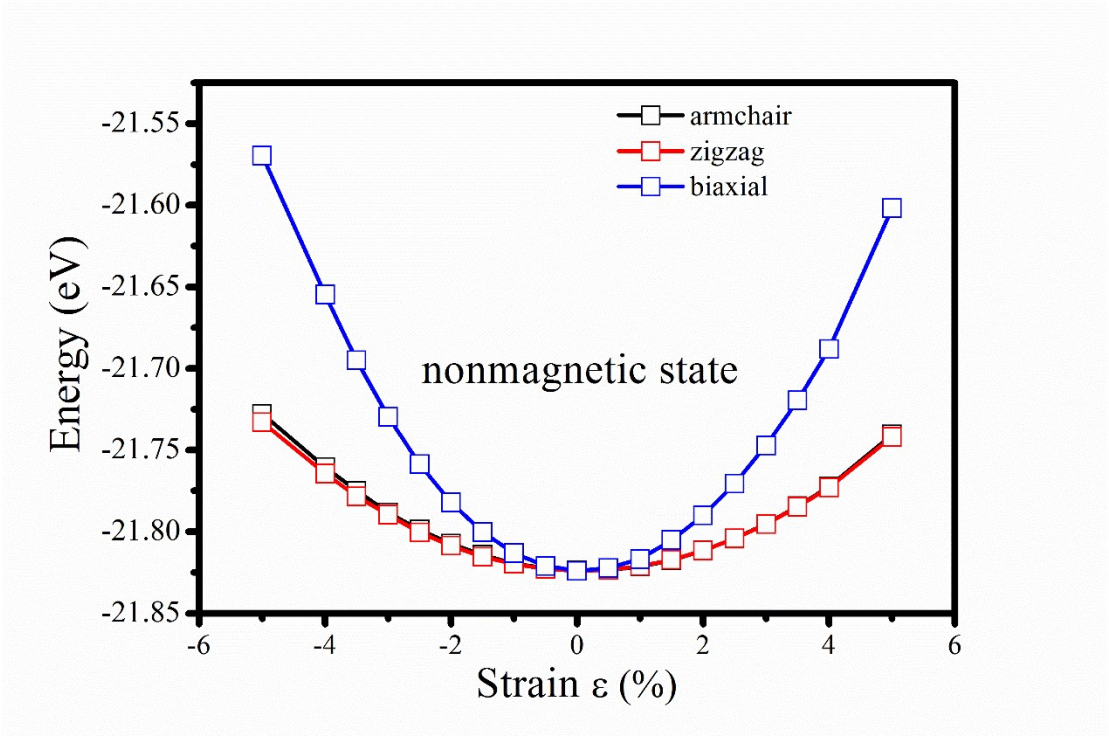

Fig.S2 The total energy of structures of nonmagnetic monolayer $FeCl_2$ depend on the strain (armchair, zigzag and biaxial). The no-strain structure is the lowest energy stable state.

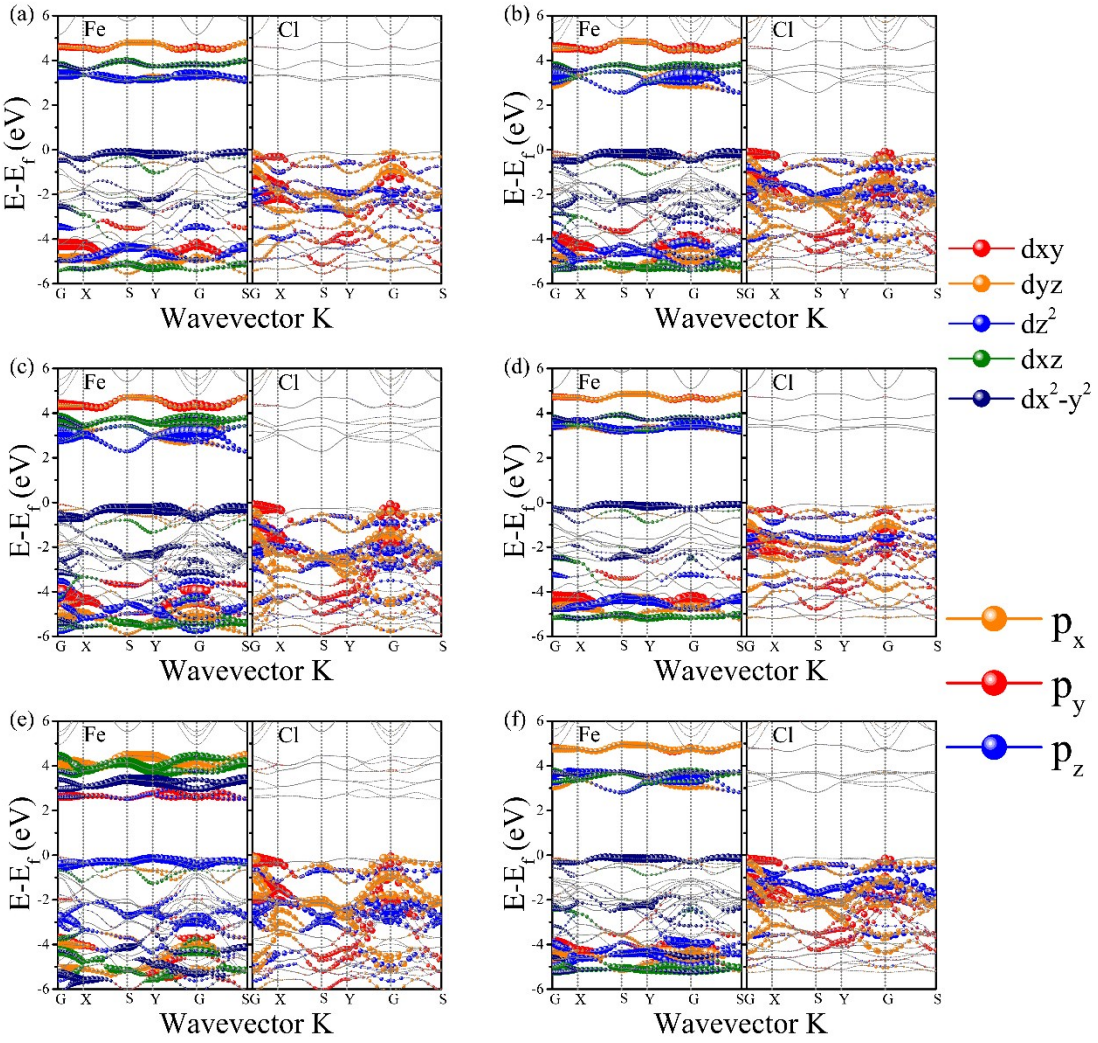

Fig.S3 Orbital projected energy bands of (a) -5% armchair, (b) +5% armchair, (c) -5% zigzag, (d) +5% zigzag, (e) -5% biaxial and (f) +5% biaxial strains. The insulator properties were found no changing by strains.

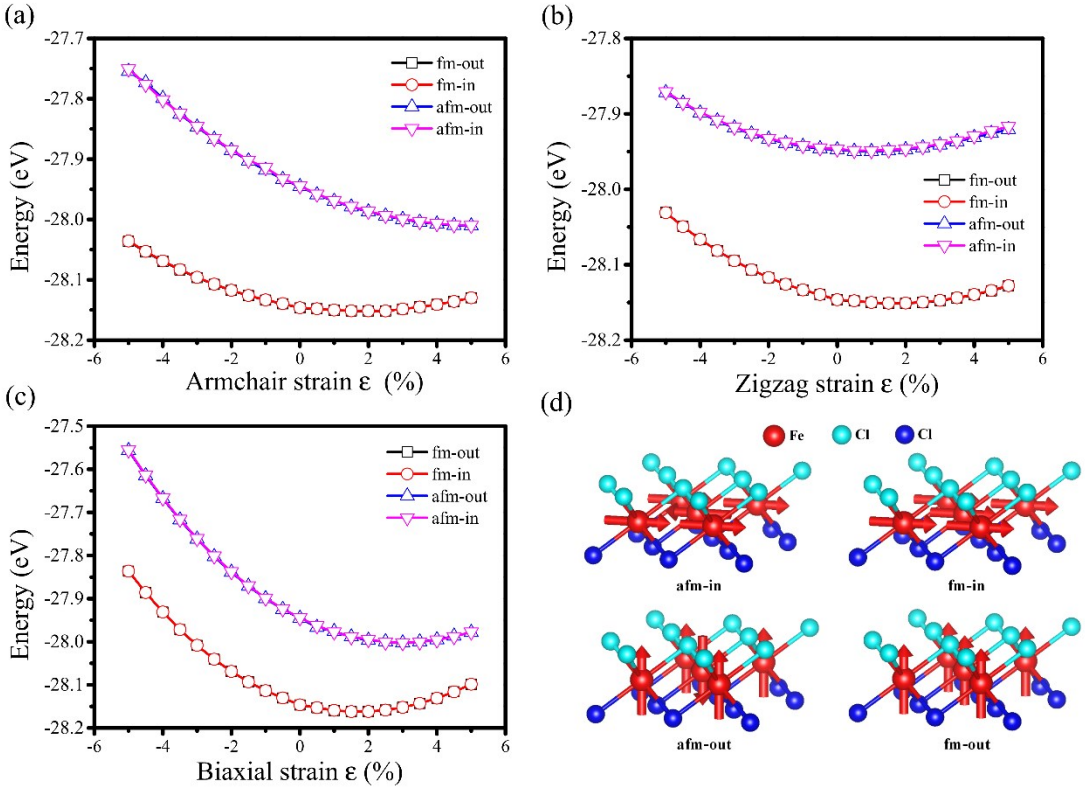

Fig.S4 The energy without U of four magnetic states dependence of (a) armchair strain , (b) zigzag strain and (c) biaxial strain. (d) The four magnetic states sketch

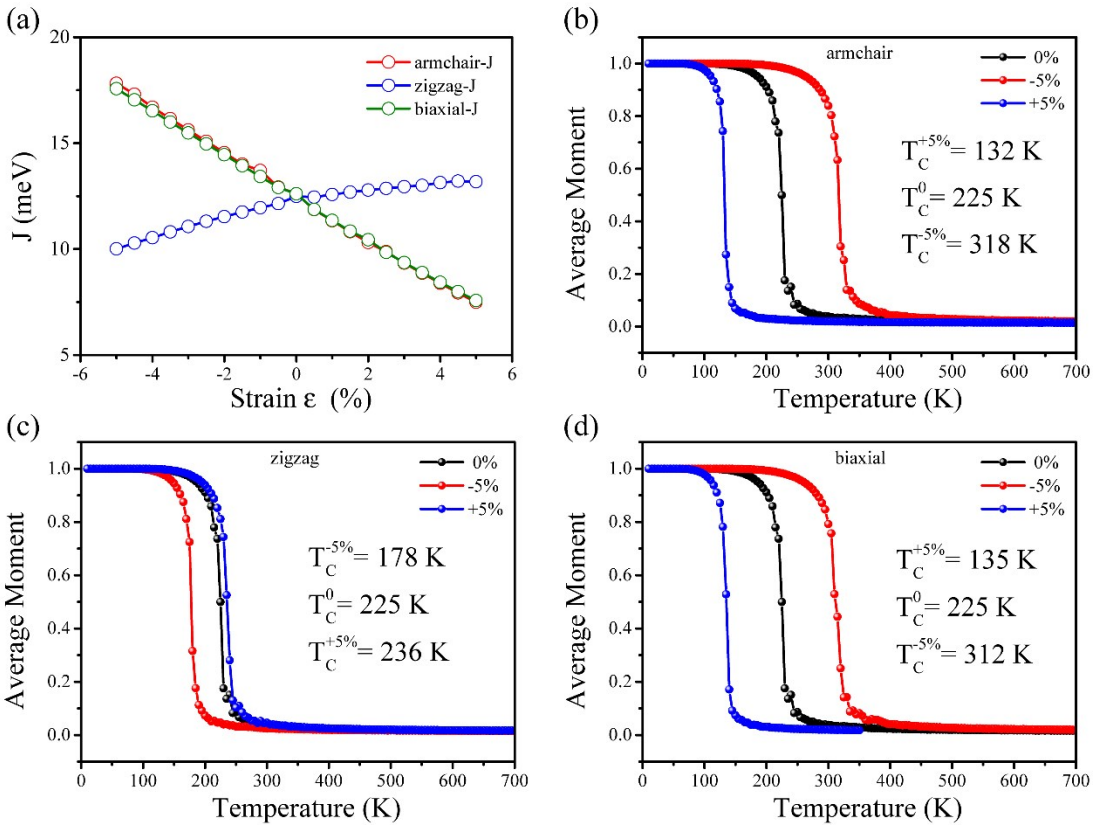

Fig.S5 (a) The magnetic exchange parameter J dependence of strains from calculations without U. Monte Carlo simulations of (b) armchair strain, (c) zigzag strain and (d) biaxial strain. The M-T curves of ±5% and 0% structure are exhibited.

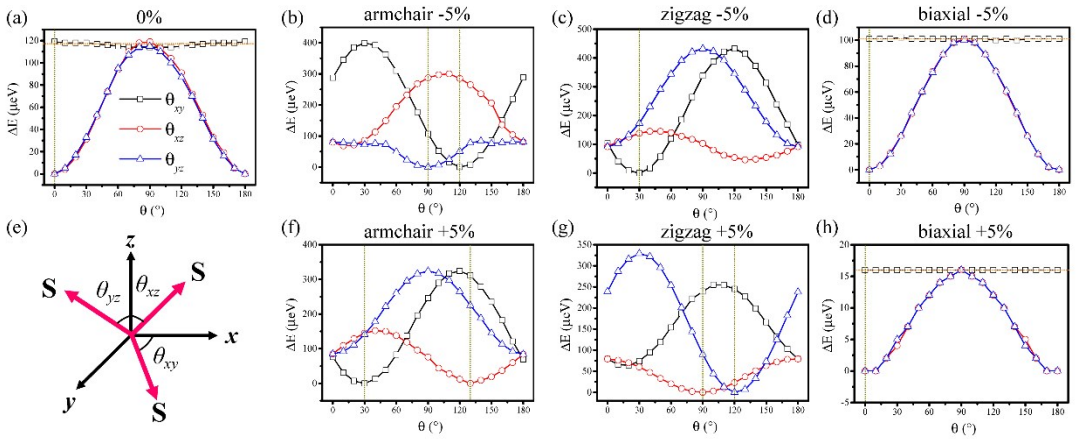

Fig.S6 The magnetoanisotropy energy dependence of the magnetic moment angles with (a) 0%, (b) -5% armchair, (c) -5% zigzag, (d) -5% biaxial, (f) +5% armchair, (g) +5% zigzag and (h) +5% biaxial strain. The magnetic moment angles are identified as (e). The magnetic easy-axial and easy-plane are presented by dotted lines. All the energy are calculated without the Hubbard U.

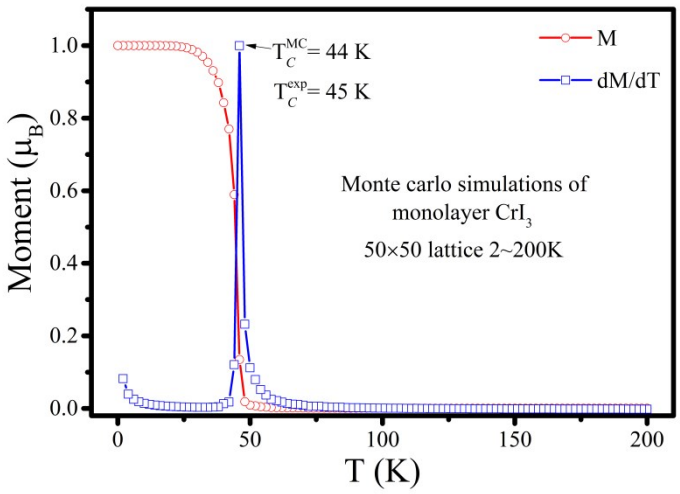

Fig.S7 The Monte Carlo simulation of the monolayer CrI_3.