Supplementary Material for "Theoretical investigation altermagnetic materials with tunable valley polarization in monolayer Nb_2Cl_2 "

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I. THE NÉEL TEMPERATURE CALCULATION

We estimate the Néel temperature for monolayer Nb_2Cl_2 by using classical Monte Carlo simulations based on the two-dimensional square lattice Heisenberg model with single-ion anisotropy,

$$H = \sum_{<i,j>} J_1 S_i \cdot S_j + \sum_{<<i,j>>} J_2 S_i \cdot S_j + \sum_{<<i,j>>} J_2' S_i \cdot S_j + A \sum_i (S_i^z)^2 \tag{1}$$

where S_i represents the spin on the i site, J_1 is the nearest exchange interaction parameter, and J_2 and J_2' are the next-nearest exchange interaction parameters with the Nb-Nb channel and Nb-Cl-Nb channel, respectively[see Fig. S1(b)]. A is the single-ion magnetic anisotropy with easy-magnetization axis.

TABLE S1: The parameters J (meV) in Eq. 1 for monolayer Nb_2Cl_2 with |S| = 1/2.

J_1^{xx}	5.931	J_2^{xx}	1.294	$J_2'^{xx}$	0.725
J_1^{yy}	5.930	J_2^{yy}	1.302	$J_2'^{yy}$	0.734
J_1^{zz}	5.903	J_2^{zz}	1.347	$J_2'^{zz}$	0.786

We use the four-state method to calculate the exchange interaction parameters in Eq. 1, which are shown in Tab. S1. The magnetocrystalline anisotropy energies are 0.393 meV for monolayer Nb_2Cl_2, respectively. After performing Monte Carlo simulations by using the

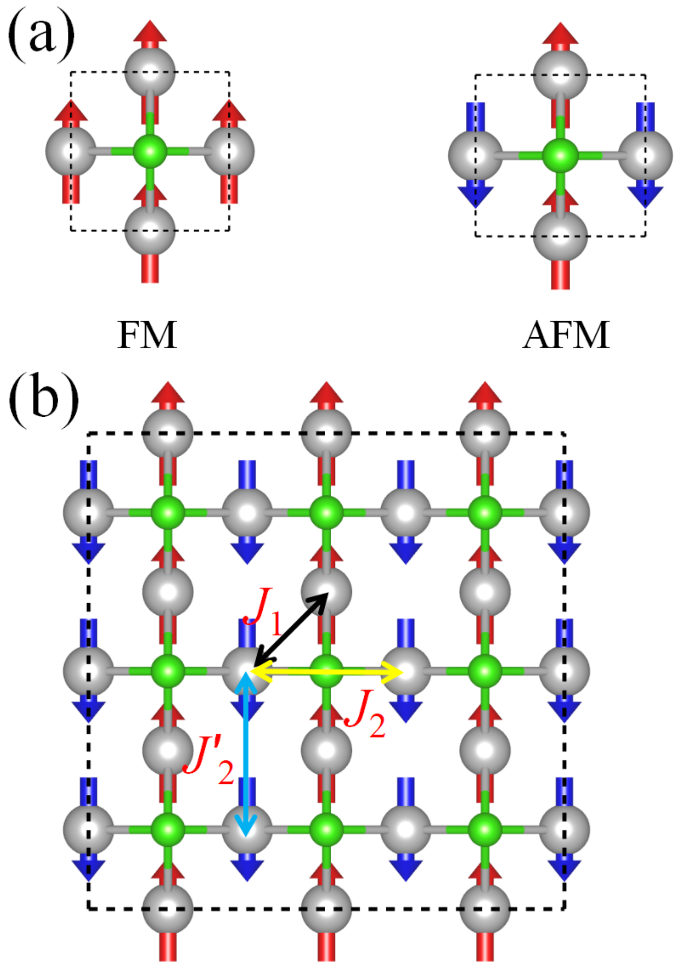

FIG. S1: Two magnetic configurations: ferromagnetic state (a) and antiferromagnetic state (b). (c) The method for determining the exchange parameter J in the antiferromagnetic $3 \times 3 \times 1$ supercell.

MCSOLVER, the resultant Néel temperature can extract from the peak of the specific-heat capacity, which is 58 K, respectively

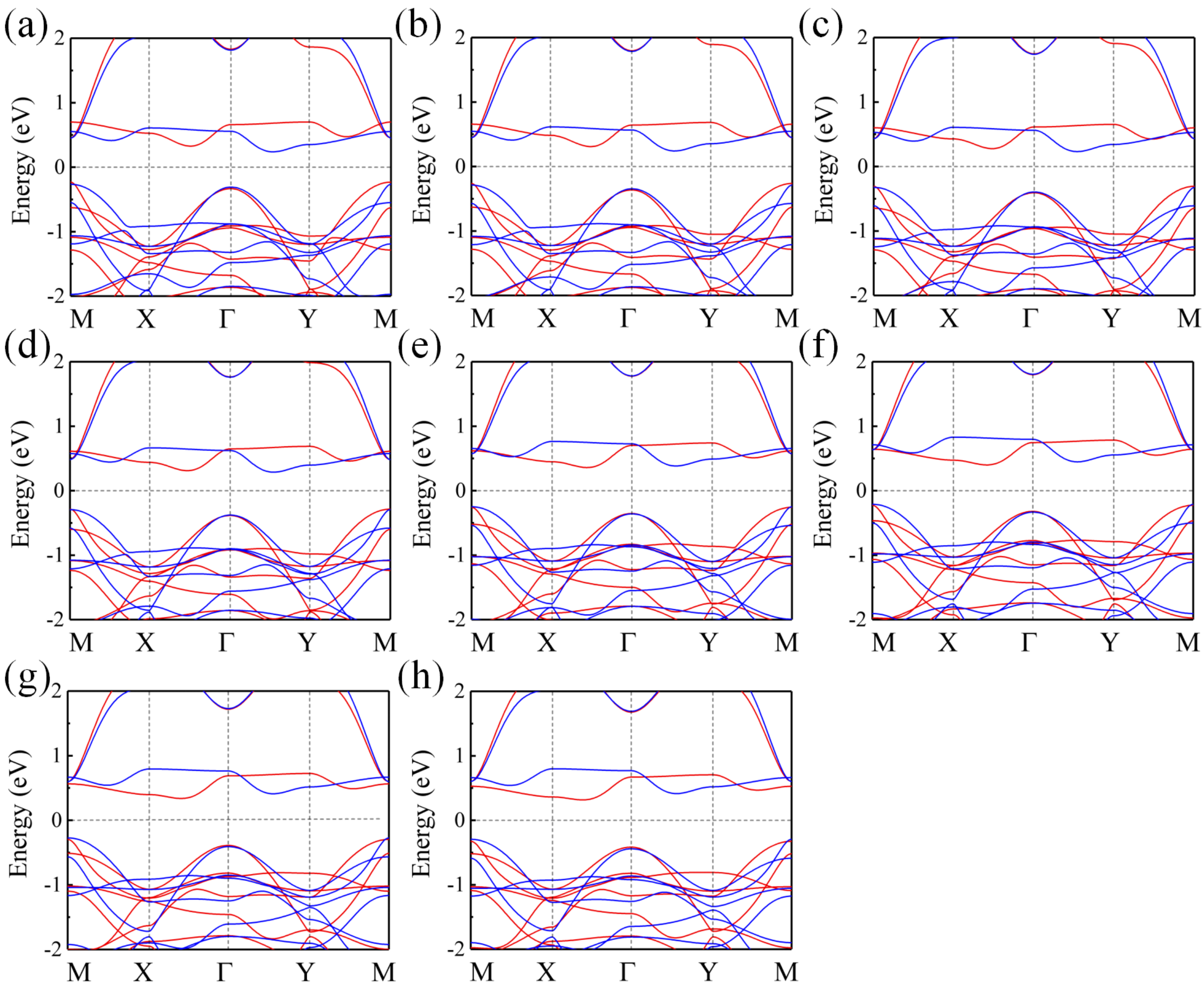

FIG. S2: Band structures without SOC at strain ε = -4% (a), -3% (b), -2% (c), -1% (d), +1% (e), +2% (f), +3% (g) and +4% (h).

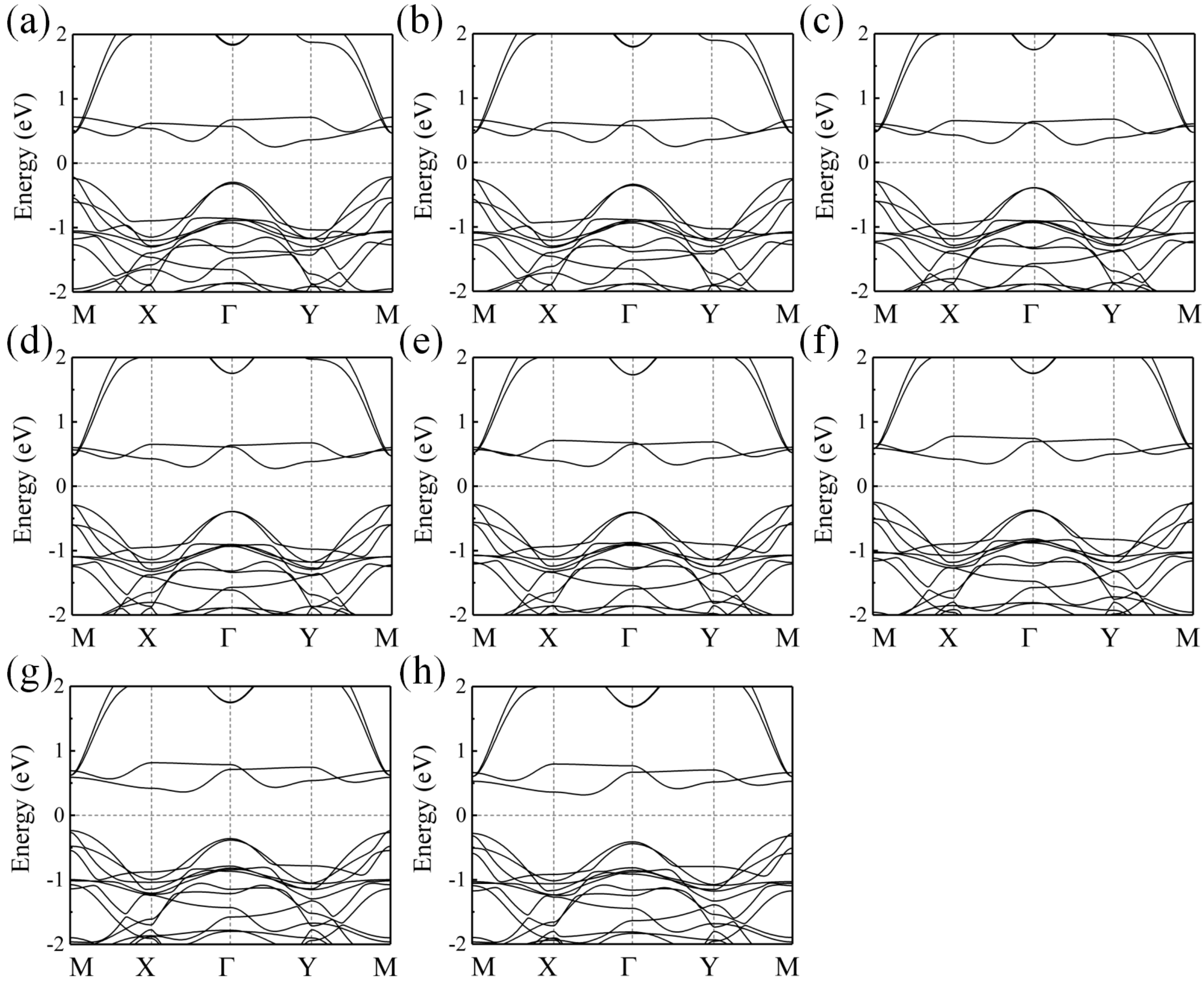

FIG. S3: Band structures with SOC at strain ε = -4% (a), -3% (b), -2% (c), -1% (d), +1% (e), +2% (f), +3% (g) and +4% (h).

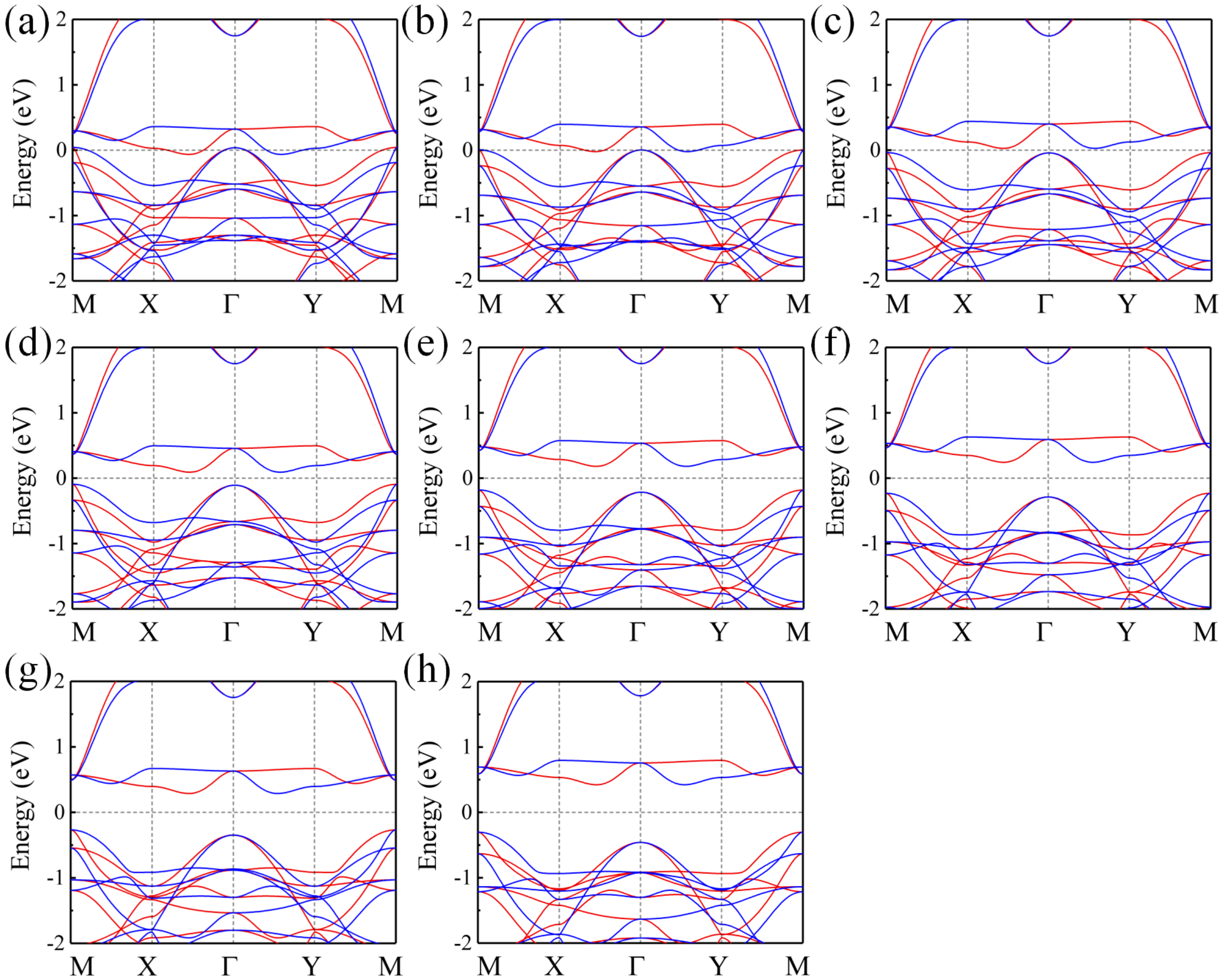

FIG. S4: Band structures without SOC at U = 0 eV (a), 0.3 eV (b), 0.6 eV (c), 1.0 eV (d), 1.6 eV (e), 2.0 eV (f), 2.3 eV (g) and 3.0 eV (h).

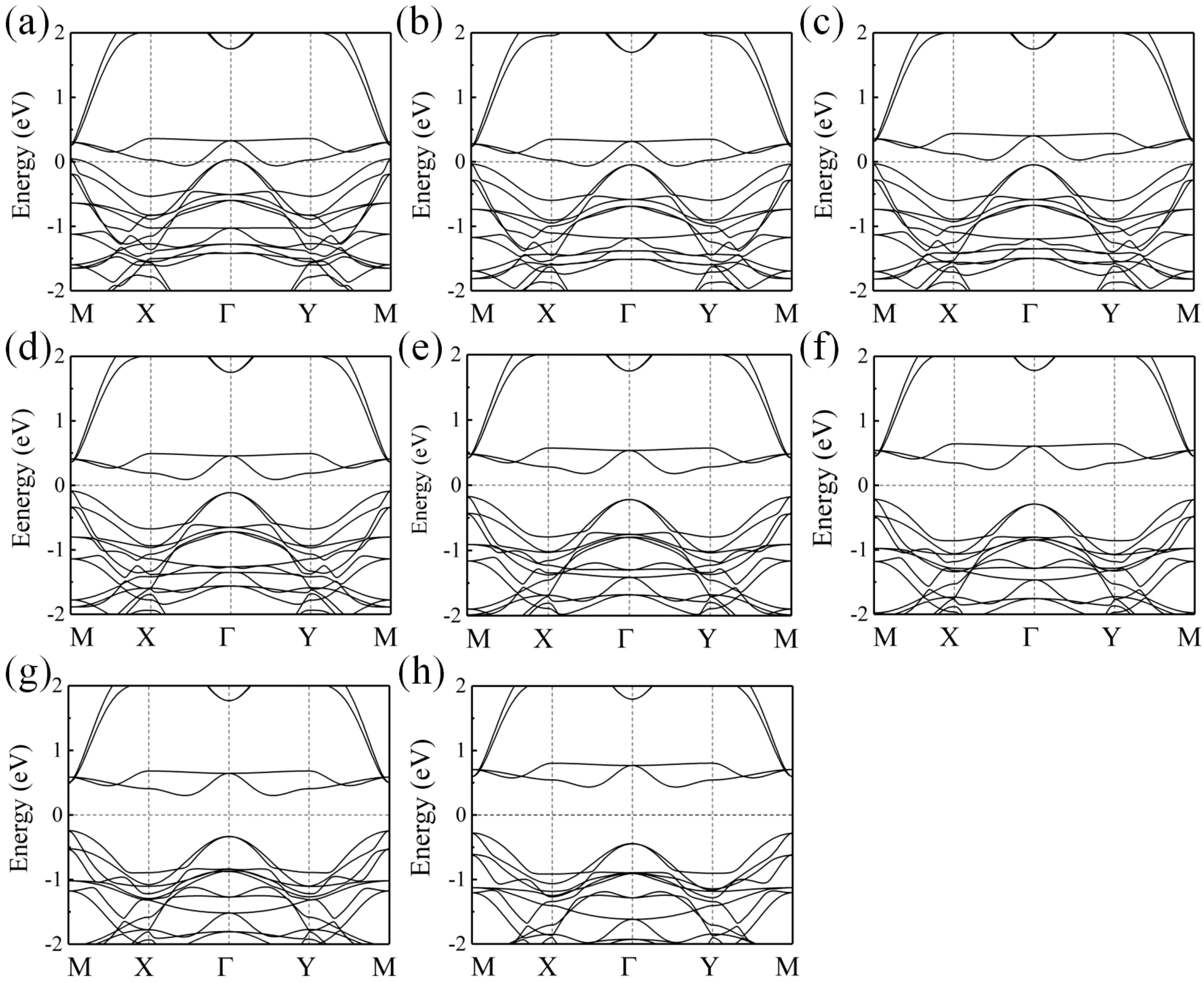

FIG. S5: Band structures with SOC at U = 0 eV (a), 0.3 eV (b), 0.6 eV (c), 1.0 eV (d), 1.6 eV (e), 2.0 eV (f), 2.3 eV (g) and 3.0 eV (h).

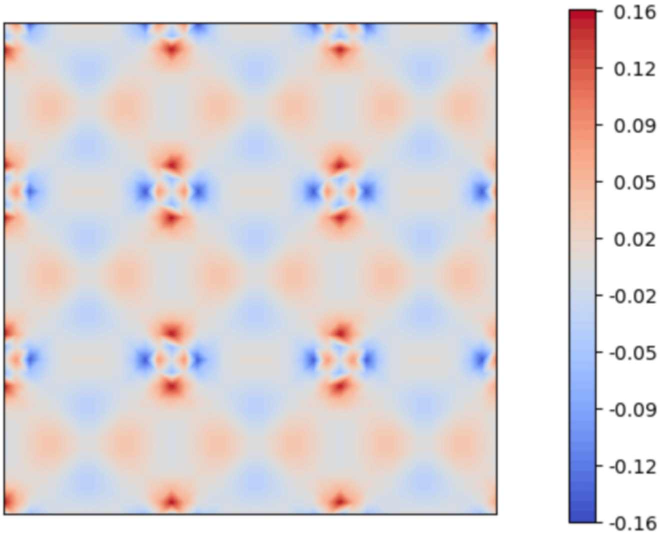

FIG. S6: The Berry curvature for monolayer Nb_2Cl_2 along the whole Brillouin zone at U = 2.5 eV.

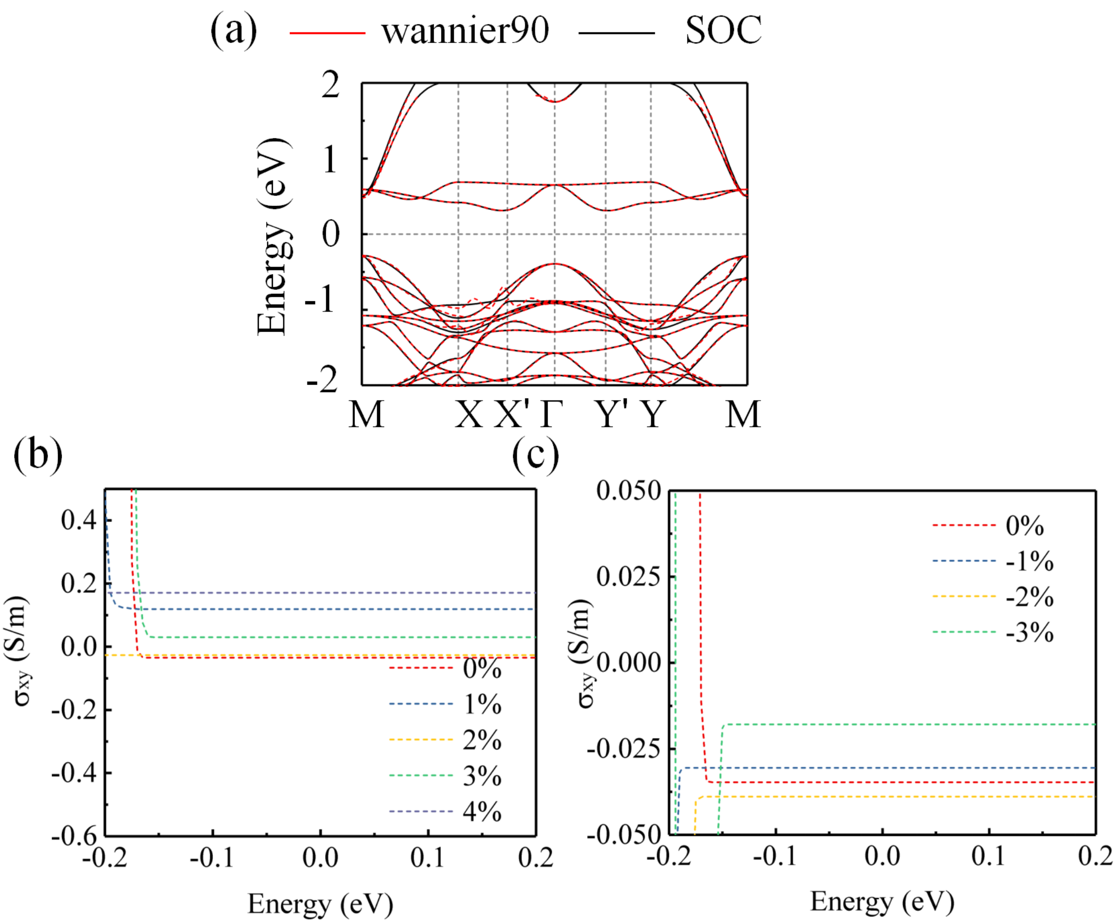

FIG. S7: The Berry curvature for monolayer Nb_2Cl_2 along the whole Brillouin zone at U = 2.5 eV.

Here, under the spin-orbit coupling (SOC) effect we use the Nb d-orbitals and fit the Wannier functions with the Wannier90 software[1]. As shown in Fig.S7(a), the red line near the Fermi level are the bands fitted by Wannier90, while the black line are the bands calculated with VASP. By constructing the Wannier Hamiltonian from the Wannier functions, we then use WannierTools[2] to compute the spin Hall conductance, as shown in Fig.S7(b)-(c). It can be seen that in the energy range from -0.2 eV to 0.2 eV, the system exhibits a very small spin Hall conductance, and with increasing strain, the spin Hall conductance becomes larger than in the unstrained.

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