Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

(Supplementary Information)

Atomic-thin layer of Ru/MoS_2 heterostructure: structural, electronic, and magnetic properties

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1. The atomic structures of 4×4 supercell for single and 5×5 supercell for double and trifoliate Ru atoms adsorbed on MoS_2. A 3×3×1 k-mesh based on gamma-centred scheme is applied for relaxation calculations and a gamma-centred 7×7×1 grid for static calculations.

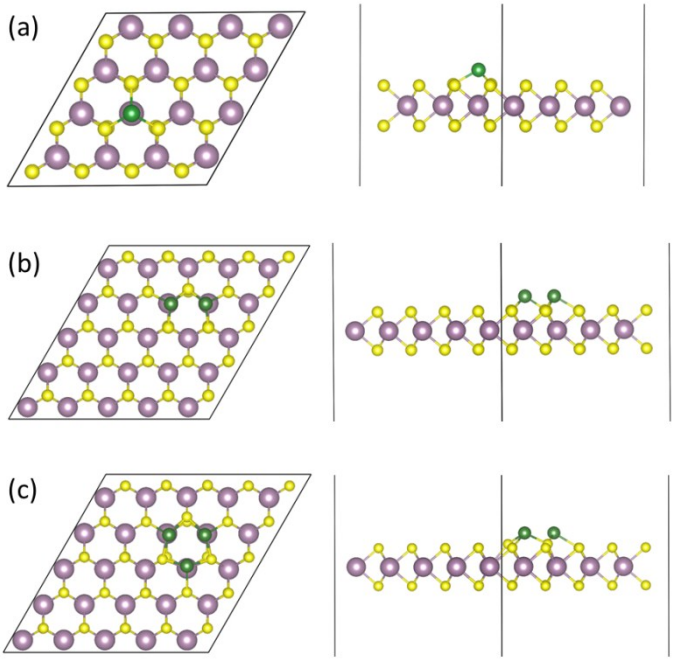

Fig. S1. The atomic structures of 4×4 supercell for single and 5×5 supercell for double and trifoliate Ru atoms adsorbed on MoS_2.

2. The lattice relaxation has been applied for the fully covered Ru/MoS_2 system, as shown in Fig. S2a. The optimized lattice constant is 3.22 Å, which is larger than 3.18 Å of pure MoS_2. Here, a 5×5×1 k-mesh based on gamma-centred scheme is applied for relaxation calculations of 2×2 supercell. A 4×4 supercell for single Ru adsorption configurations is also relaxed and the lattice constant is ~3.18 Å (see Fig. S2b).

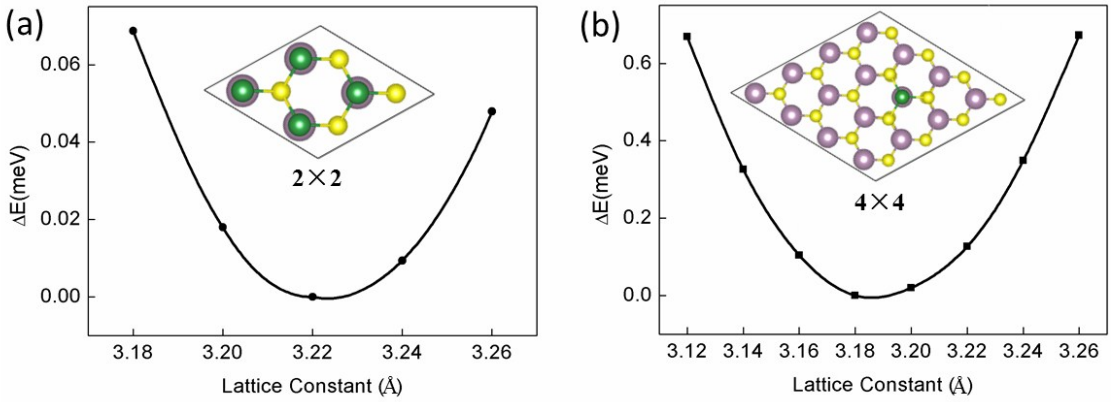

Fig. S2. The fitted line of total energy versus lattice constants, the units of lattice constants are given in angstroms.

3. A 6×6 supercell of Ru/MoS_2 layer has been constructed to calculate the FM and AFM coupling states, as shown in Fig. S3. The energy difference ($\Delta E_{\text{AFM-FM}}$) is 173meV, which has verified the accuracy of the result ($\Delta E_{\text{AFM-FM}}$ = 171meV) obtained from a 2×2 supercell.

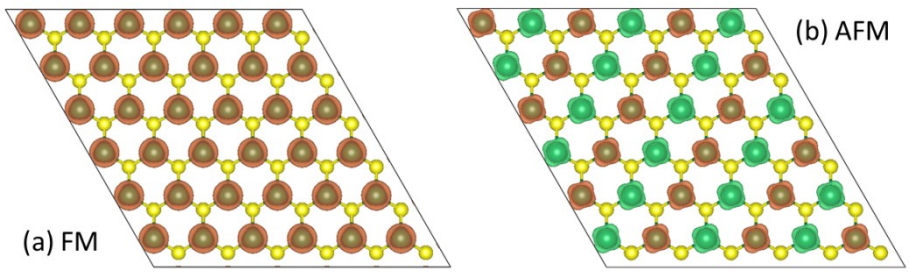

Fig. S3. Spin density of a 6×6 Ru/MoS_2 layer with FM (a) and AFM (b) coupling, the iso-value is 0.008 e/Å^3.