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

Supplementary Information

Inducing Abundant Magnetic Phases and Enhancing Magnetic Stability by Edge Modifications and Physical Regulations for NiI_2 Nanoribbons

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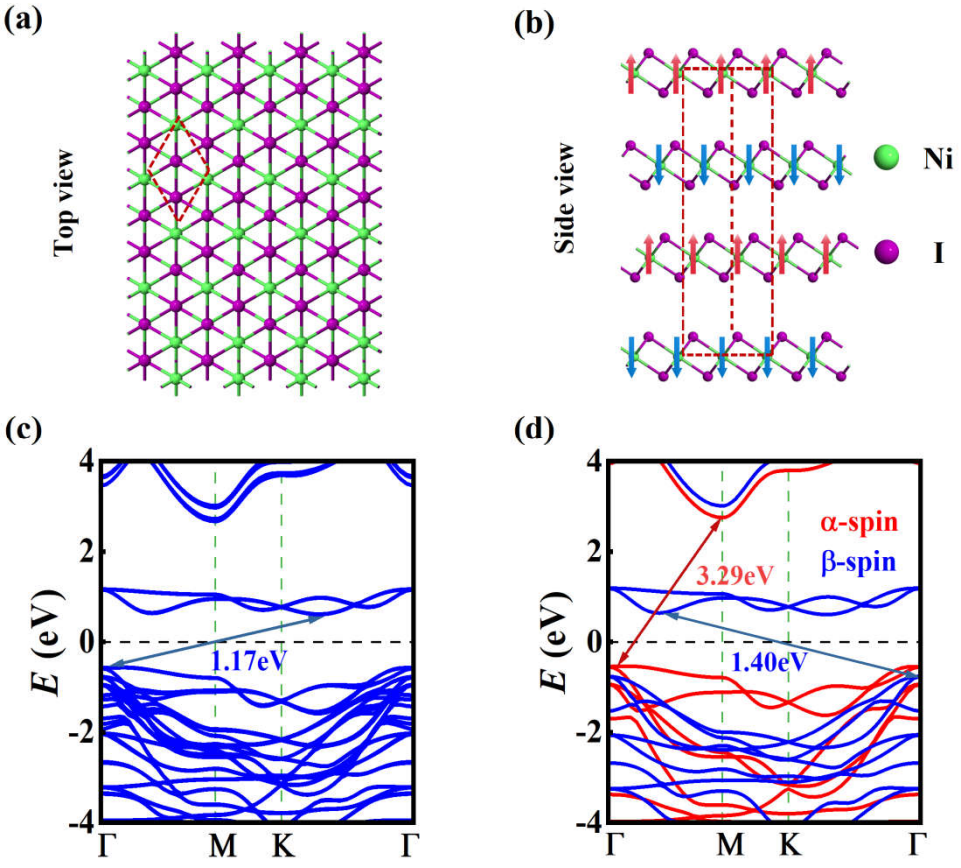

Fig. S1. (a)Top view, (b) side view and magnetic ordering of bulk NiI_2 atomic structure, in which the red dashed rhombus indicates the 1×1 unit cell. (c) Band structure of bulk NiI_2. (d) Band structure of NiI_2 monolayer.

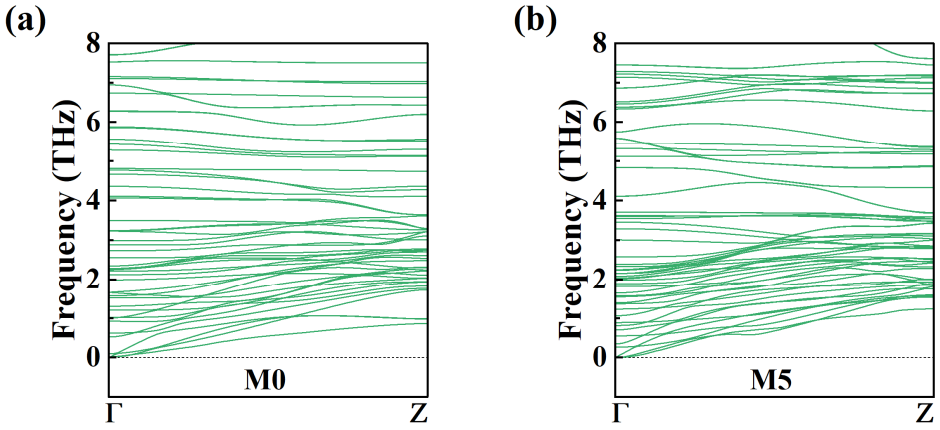

Fig. S2. Phonon dispersion for $ZNiI_2NRs$. (a) M0, (b) M5.

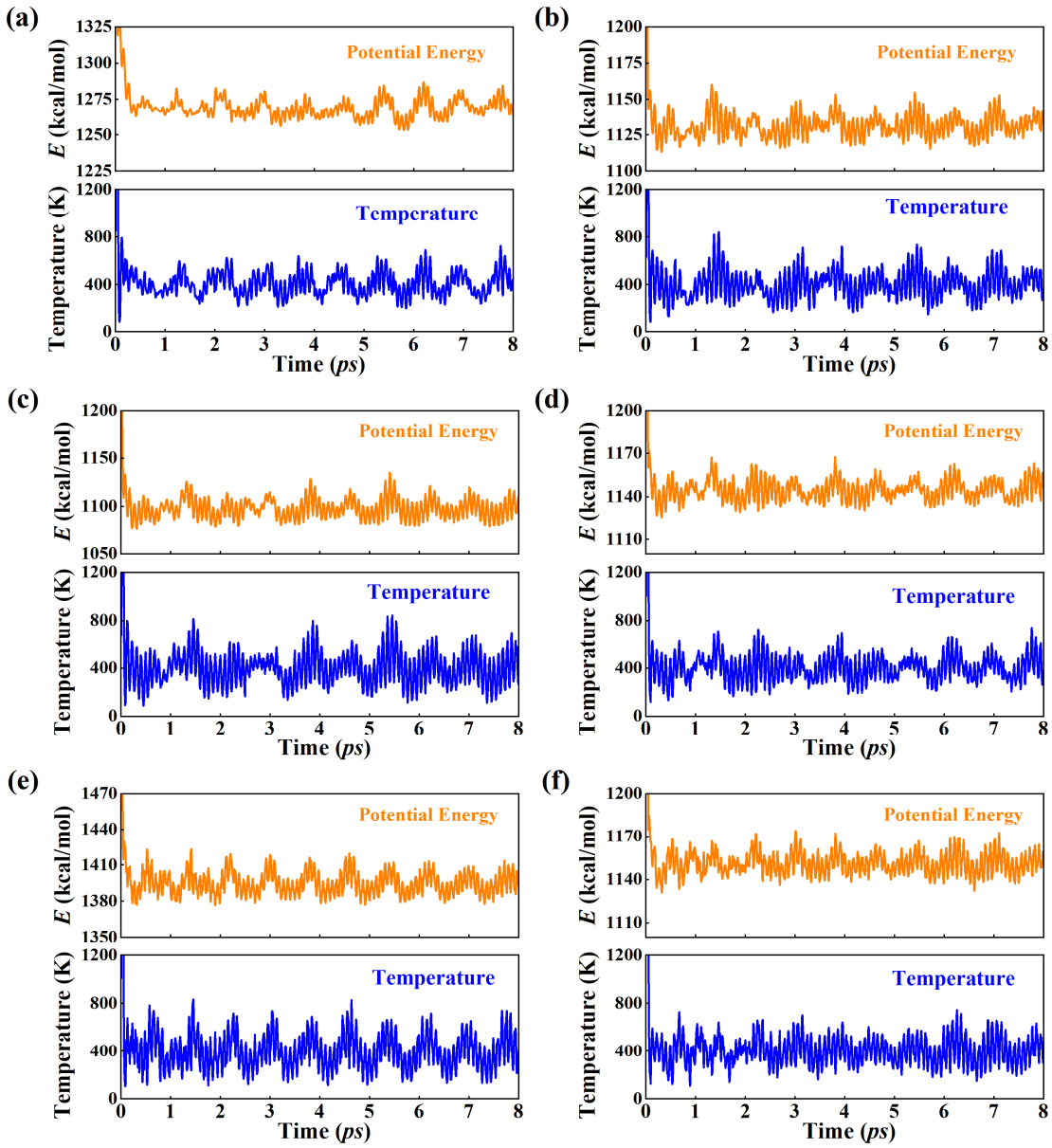

Fig. S3. Energy and temperature versus time profiles of nanoribbons in annealing molecular dynamics simulations. (a) M0, (b) M1, (c) M2, (d) M3, (e) M4, and (f) M5.

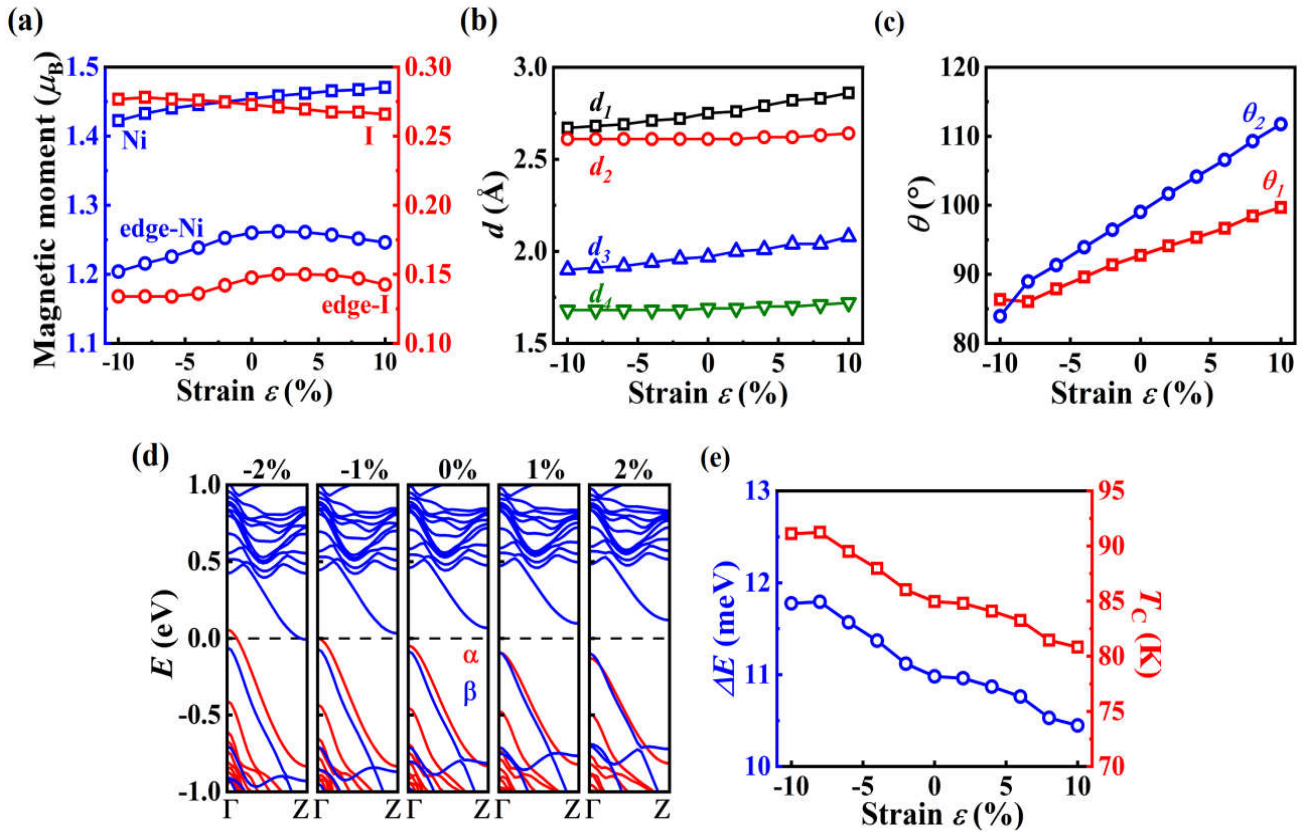

Fig. S4. For M3. (a) Averaged magnetic moment for whole ribbon and edged Ni and I atoms in the FM state versus strain, (b) edged atom bond lengths d_1, d_2, d_3, and d_4 versus strain, (c) edge atom bond angles θ_1 and θ_2 versus strain, (d) the band structure in the FM state versus strain, and (e) magnetic exchange energy ΔE and Curie temperature T_C versus strain.