Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Table 1. Dissolution Potentials (U_{diss}) and Binding Energies (E_b) of TM in TM-Nb_2C.

Metal	U_{diss} (V)	E_b (eV)
Ti	-0.25	-2.76
V	-0.16	-2.04
Mn	-0.30	-1.77
Fe	0.02	-0.94
Co	0.32	-1.21
Y	-1.20	-3.52
Zr	-0.67	-3.14
Mo	0.48	-2.04

Table S2. The calculated adsorption energy of N_2 at different sites.

Metal	ΔE_{hollow} (eV)	ΔE_{top} (eV)	ΔE_{bridge} (eV)
Fe	-2.68	-1.96	-
Co	-2.48	-1.15	-1.89
Mo	-2.35	-1.06	-1.60

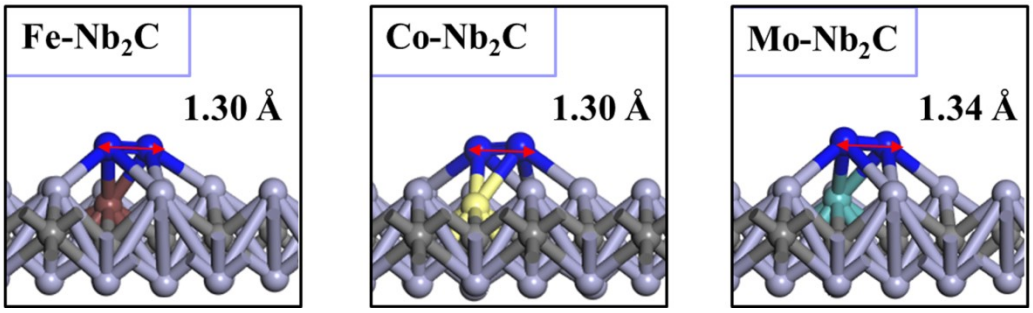

Figure S1. Optimized adsorption configurations of N_2 adsorbed on Fe-Nb_2C, Co-Nb_2C, Mo-Nb_2C.

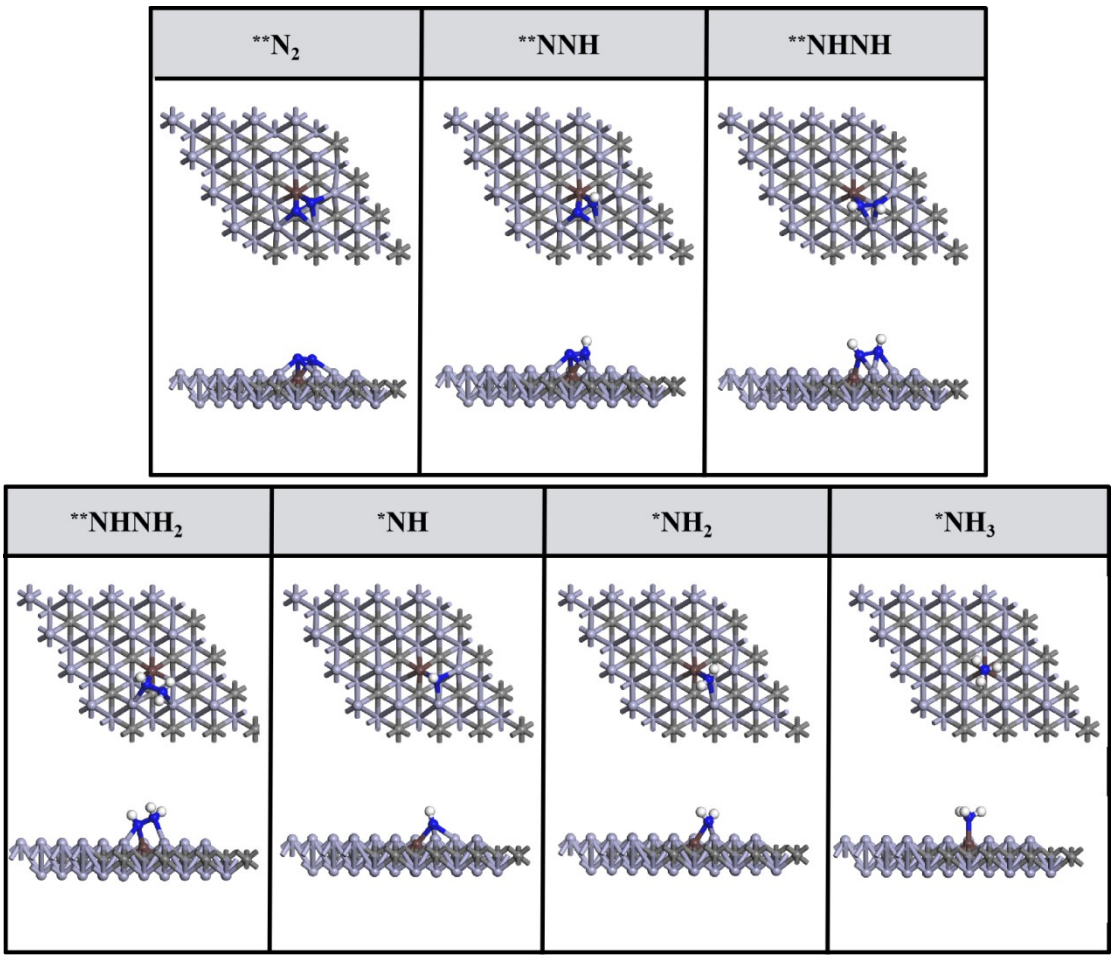

Figure S2. Geometric structure of intermediates involved in Fe-Nb_2C catalytic NRR along the mixed pathway.

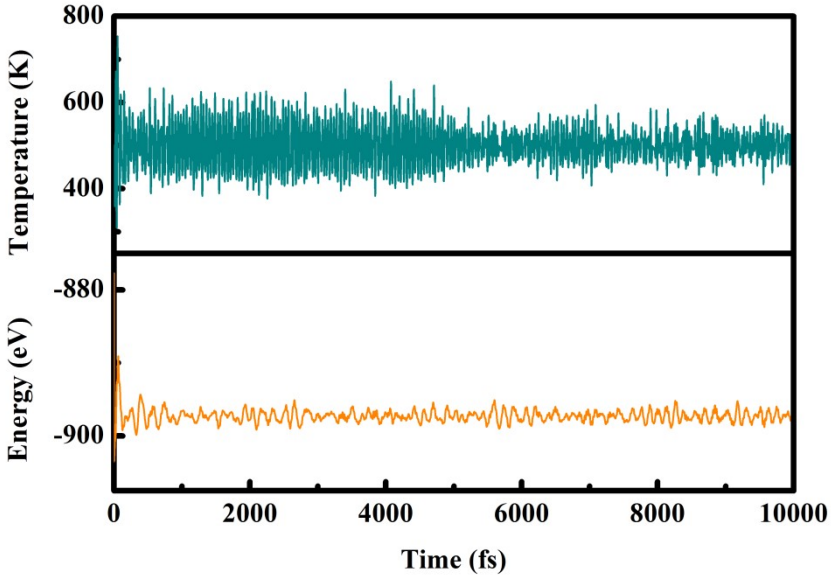

Figure S3. Variations of temperature and energy against the time for AIMD simulations of Fe-Nb_2C; the simulation is run at 500 K for 10 ps with a time step of 1 fs.

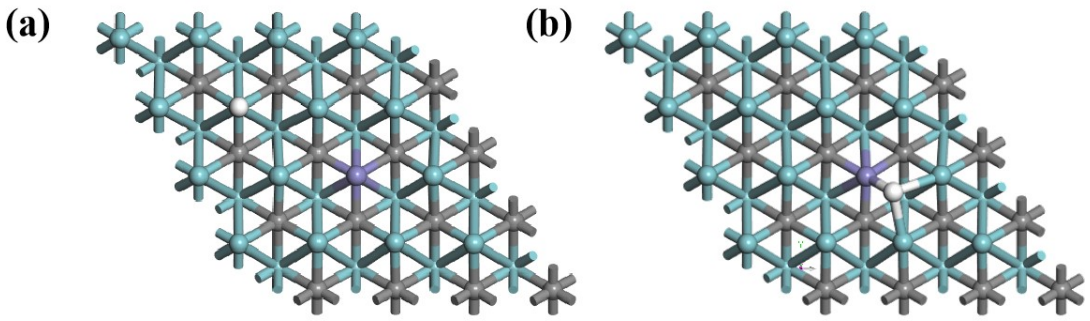

Figure S4 Geometric structures of H adsorption on Fe-Nb_2C at (a) Nb site and (b) hollow site.

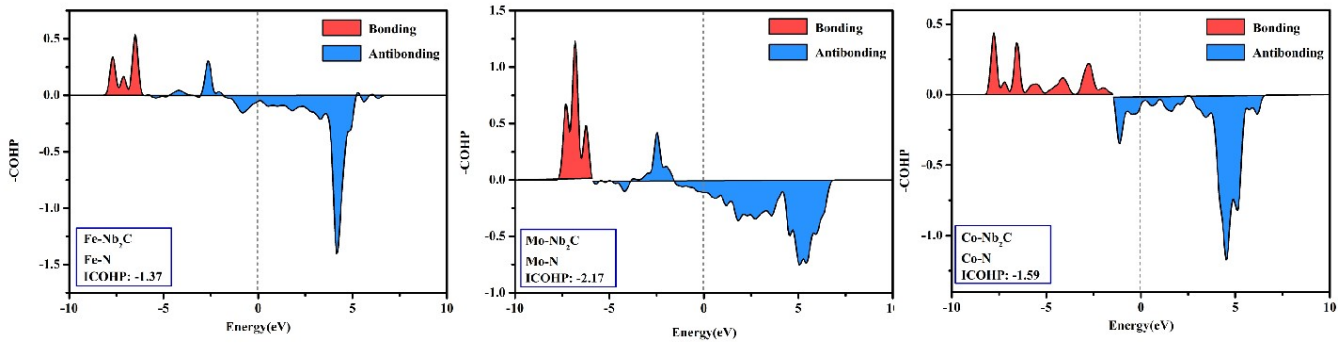

Figure S5 The crystal orbital Hamilton population (COHP) of N-N bond of free N_2 molecule, adsorbed N_2 on the Fe-Nb_2C、Mo-Nb_2C、Co-Nb_2C. The bonding and antibonding states in -COHP are depicted by red and blue, respectively.

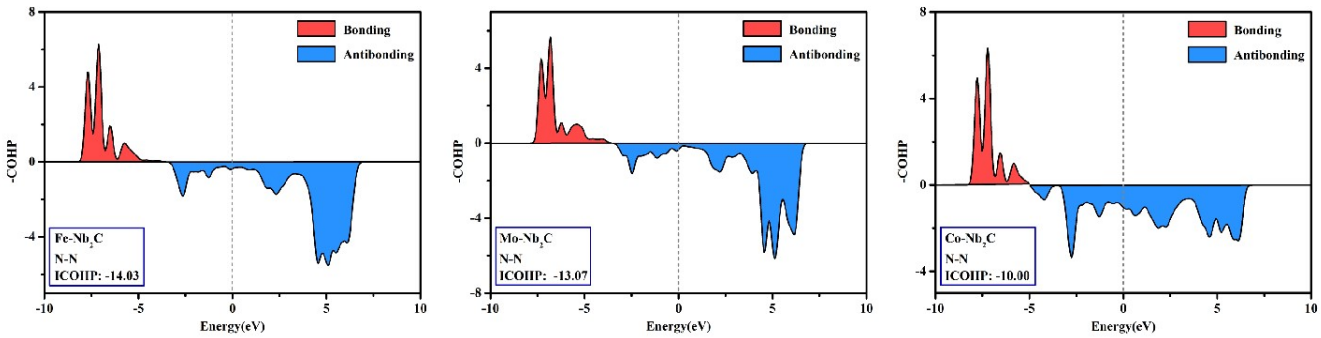

Figure S6 The crystal orbital Hamilton population (COHP) of M-N bond on the Fe-Nb_2C、Mo-Nb_2C、Co-Nb_2C. The bonding and antibonding states in -COHP are depicted by red and blue, respectively.