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

Supporting Information

Single transition metal atoms anchored on C_2N monolayer as efficient catalysts for hydrazine electrooxidation

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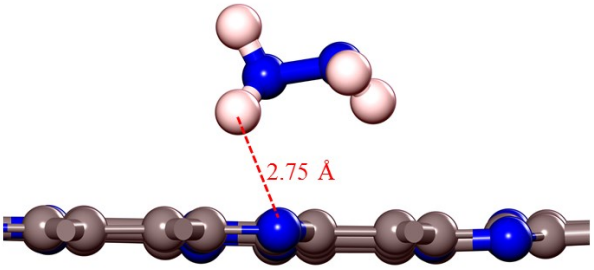

Fig. S1. The optimized adsorption configuration of N_2H_4 molecule on pristine C_2N monolayer.

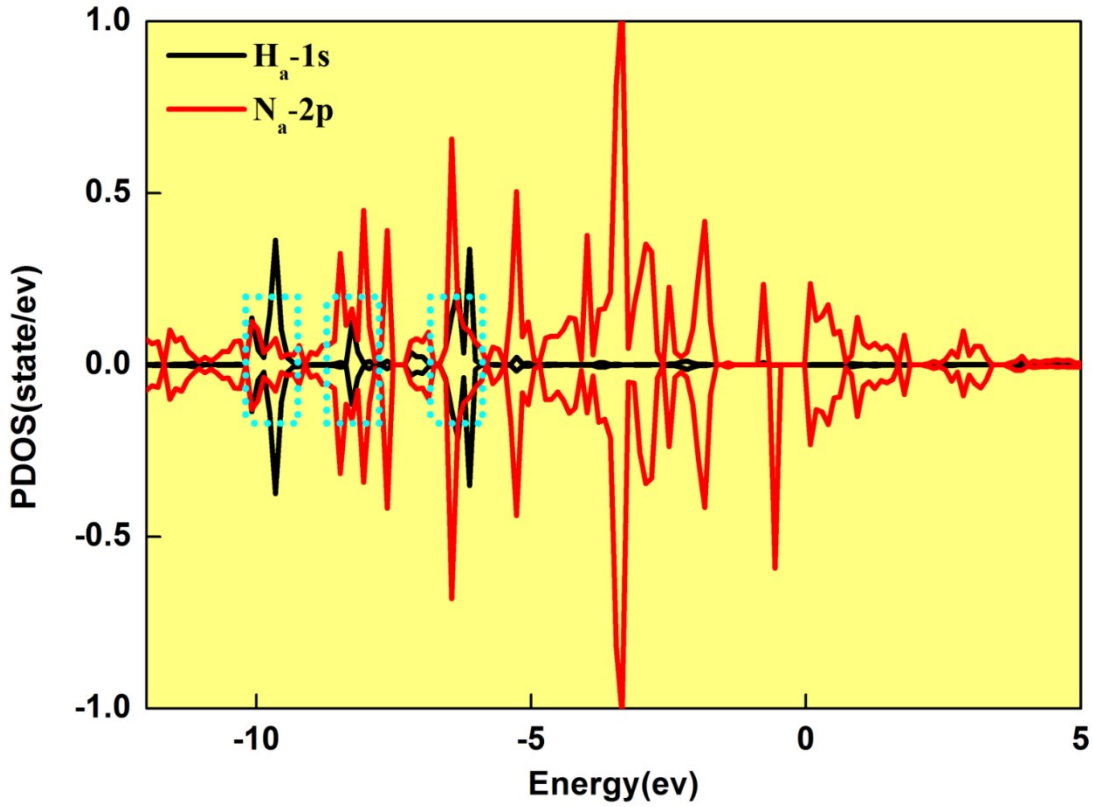

Fig. S2. The computed projected density of states (PDOSs) between the H_a-1s of adsorbed $N_2H_4^*$ species and the N_a-2p orbitals of C_2N monolayer.

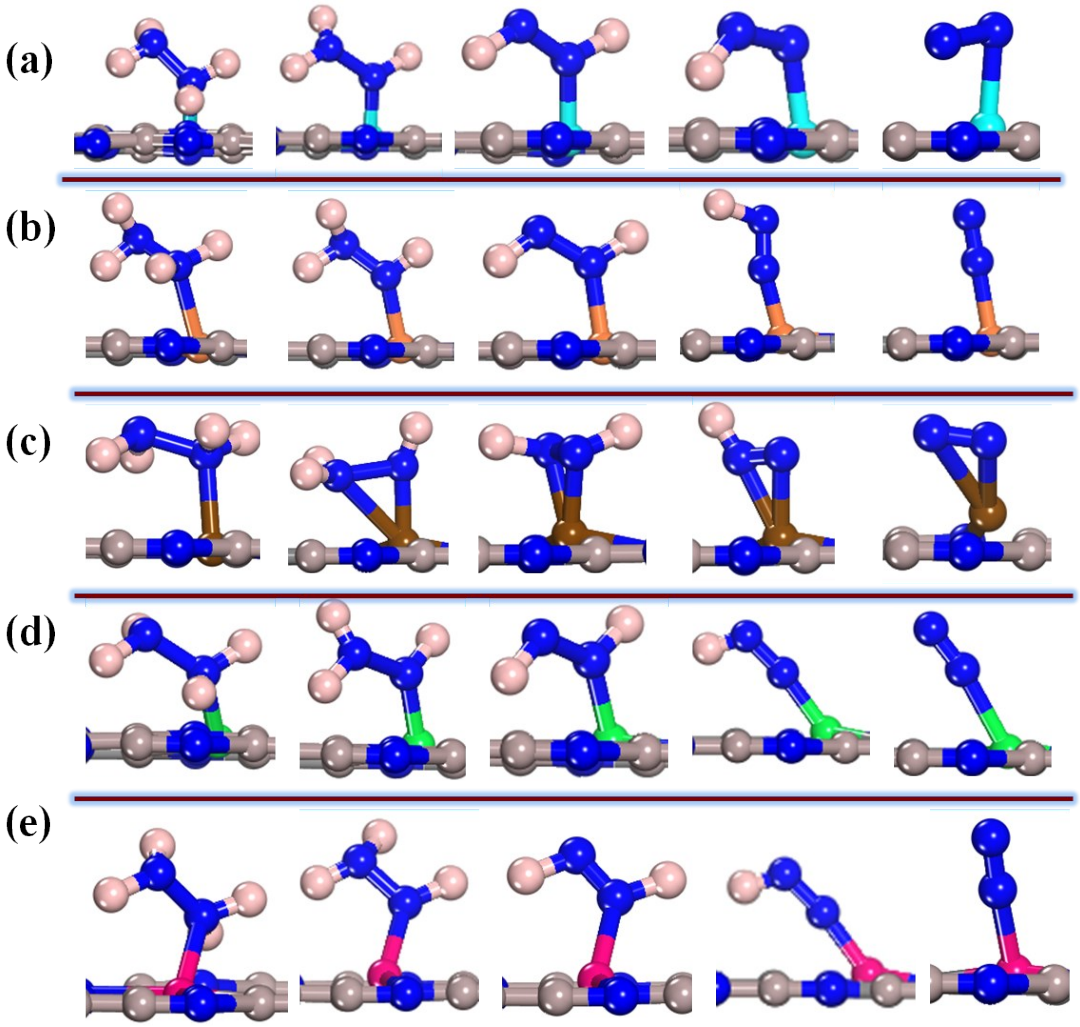

Fig. S3. The involved reaction intermediates $N_2H_4^*$, $N_2H_3^*$, $N_2H_2^*$, N_2H^*, and N_2^* species during HzOR on (a) Ru@C_2N, (b) Mo@C_2N, (c) Ti@C_2N, (d) Co@C_2N, and (e) Fe@C_2N.

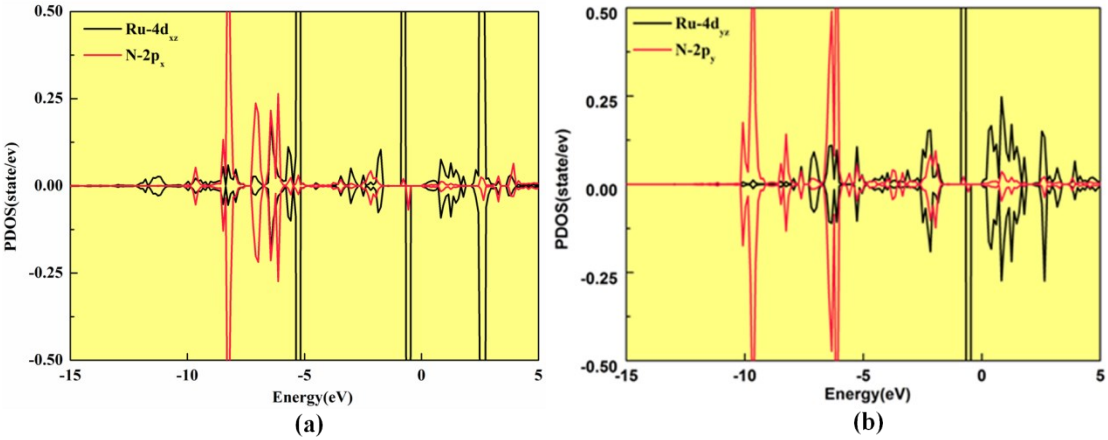

Fig. S4. The computed projected density of states (PDOSs) of (a) Ru($4d_{xz}$)-$N_2H_4^*$($2p_x$) and (b) Ru($4d_{yz}$)-$N_2H_4^*$($2p_y$) for N_2H_4 adsorption on Ru@C_2N.