Supplementary Materials

Tailoring of Three-Atom Metal Cluster Catalysts for Ammonia Synthesis

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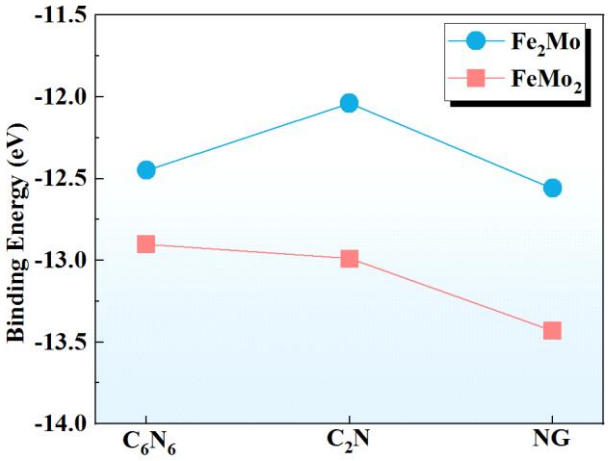

Figure S1. Binding energies of Fe_xMo_y@CN (x = 1, 2; x + y = 3).

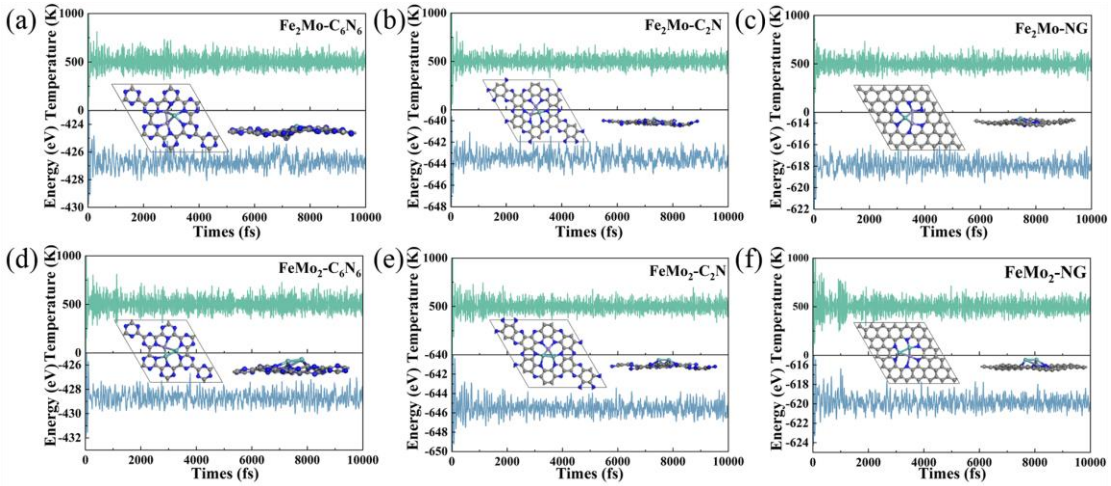

Figure S2. Variation of the total energy and temperature against time for the AIMD simulation on Fe_xMo_y-CNs.

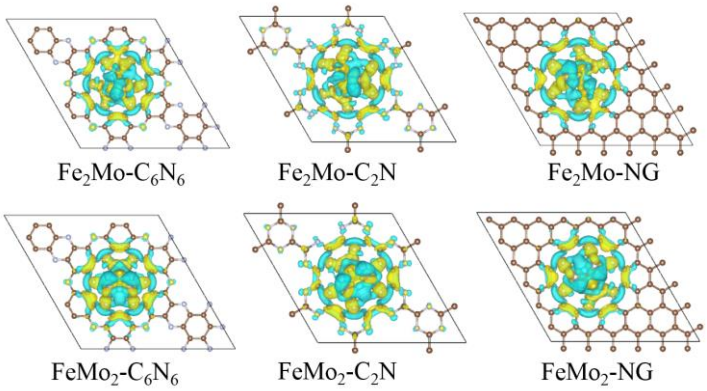

Figure S3. Charge density differences of Fe_xMo_y@CN (x = 1, 2; x + y = 3).

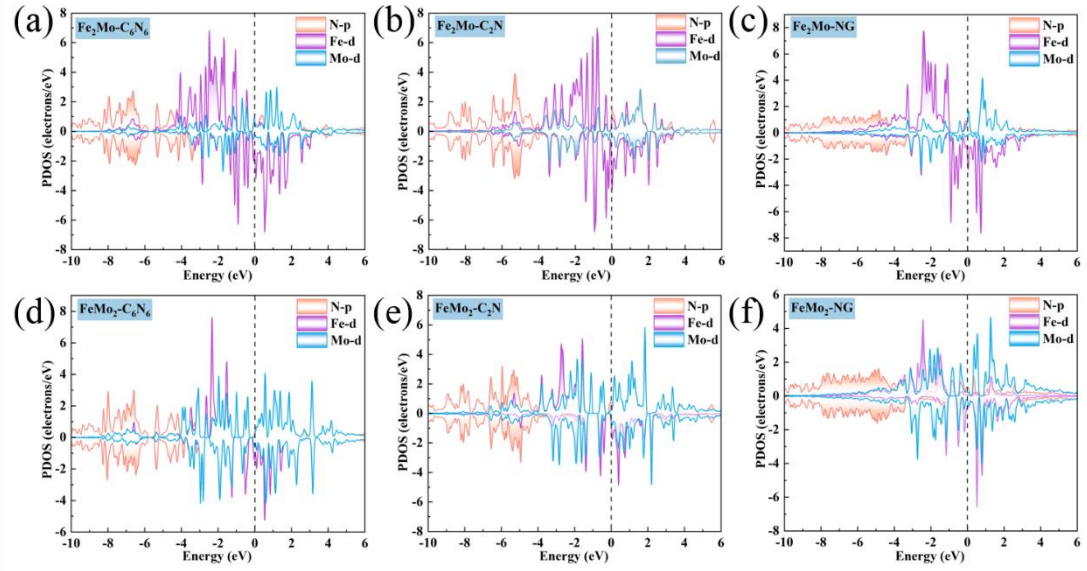

Figure S4. Computed projected density of states (PDOSs) of Fe_xMo_y-CNs.

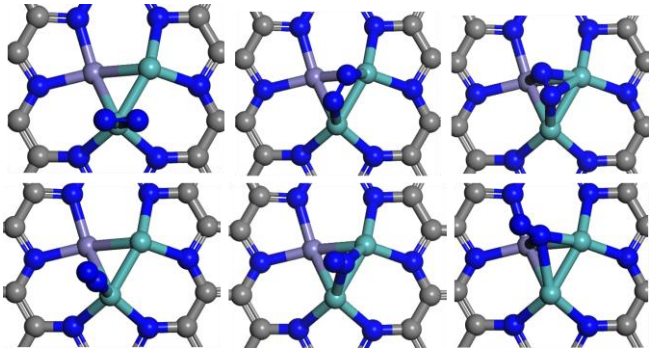

Figure S5. All possible initial N_2 adsorption configurations.

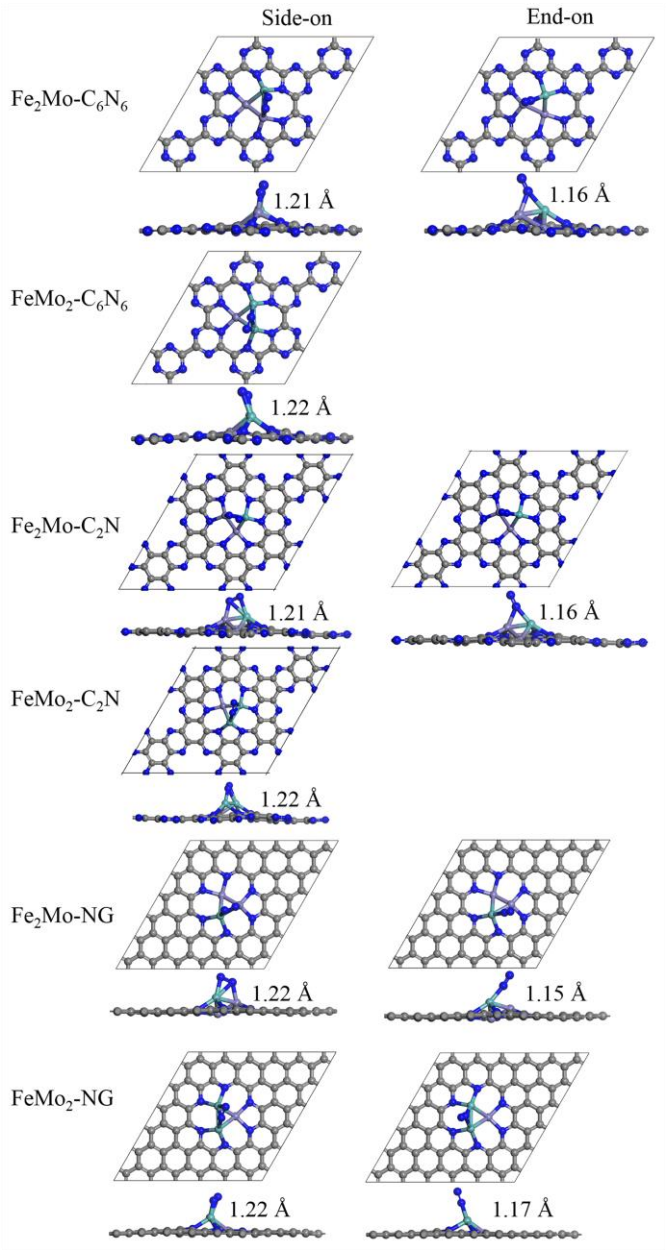

Figure S6. The configurations and bond length of N_2 adsorption on Fe_xMo_y-CNs via

end-on and side-on patterns.

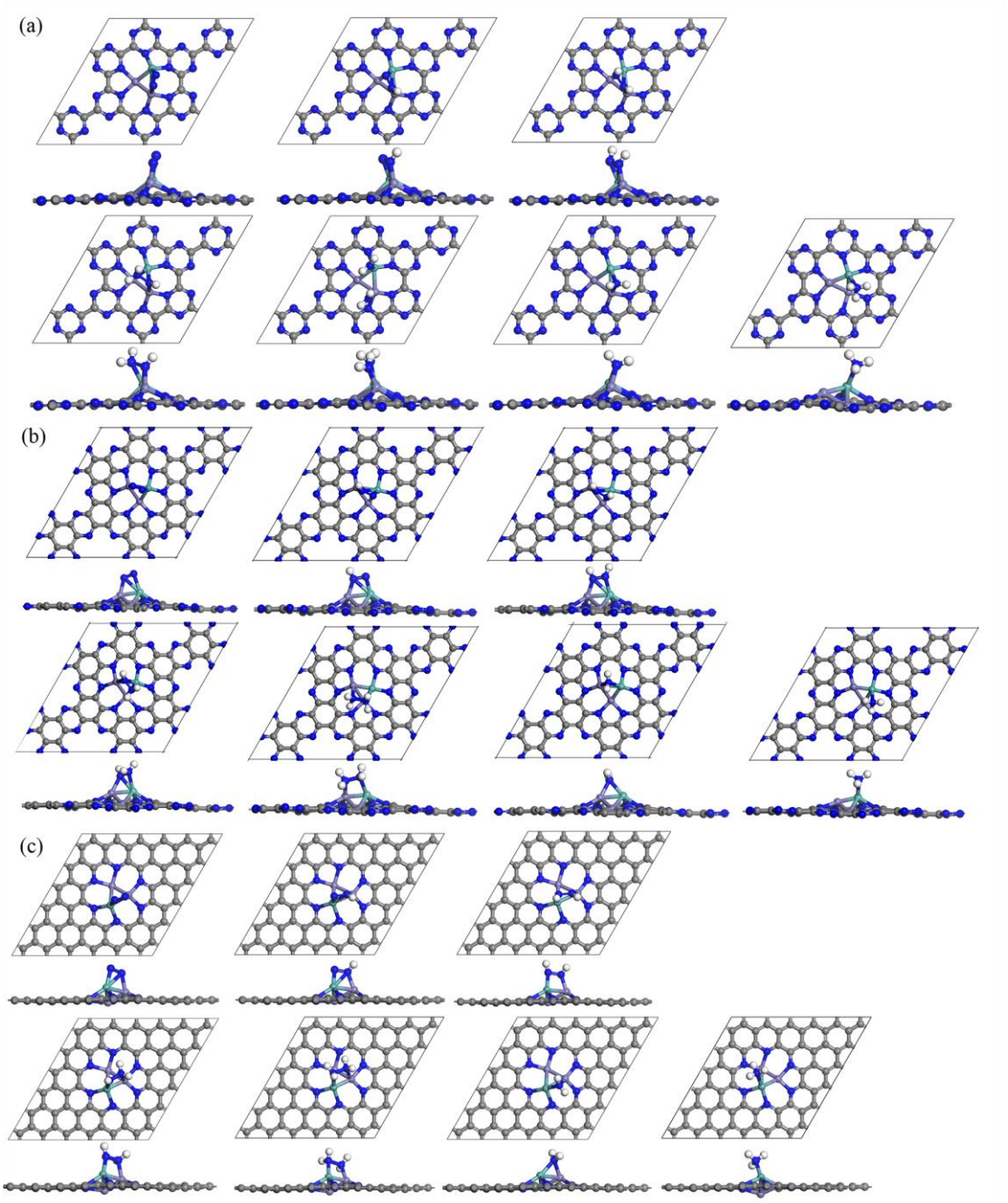

Figure S7. Corresponding geometric structures of intermediates along the enzymatic pathway on (a) Fe_2Mo-C_6N_6, (b) Fe_2Mo-C_2N, and (c) Fe_2Mo-NG.

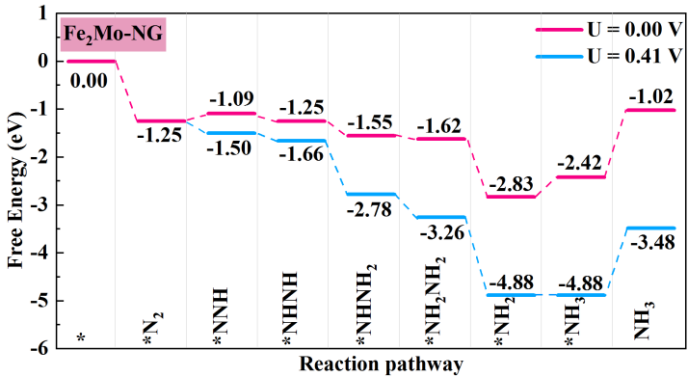

Figure S8. Free energy diagrams of NRR by considering solvation effect for enzymatic pathway on Fe_2Mo-NG.

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24 48 1 2

Direct

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