



## Article

# Single-atom anchored g-C<sub>3</sub>N<sub>4</sub> monolayer as efficient catalysts for nitrogen reduction reaction

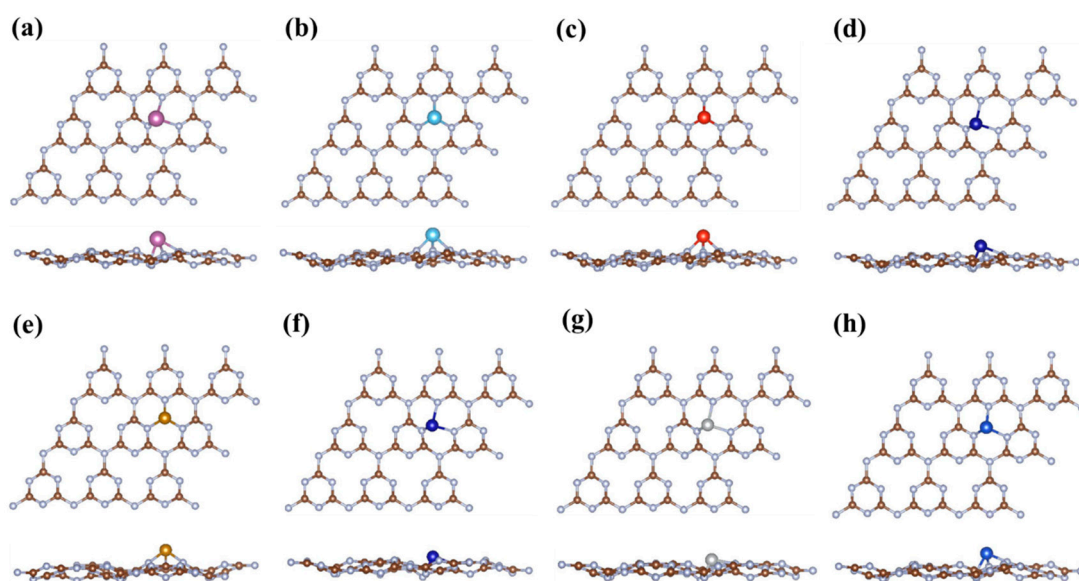
Huadou Chai <sup>a,b</sup>, Weiguang Chen <sup>b</sup>, Zhen Feng <sup>c</sup>, Yi Li <sup>b</sup>, Mingyu Zhao <sup>b</sup> and Jinlei Shi <sup>b</sup>, Yanan Tan <sup>b,\*</sup>, Xianqi Dai <sup>a,\*</sup>

<sup>a</sup> School of Physics, Henan Normal University, Xinxiang, Henan 453007, China

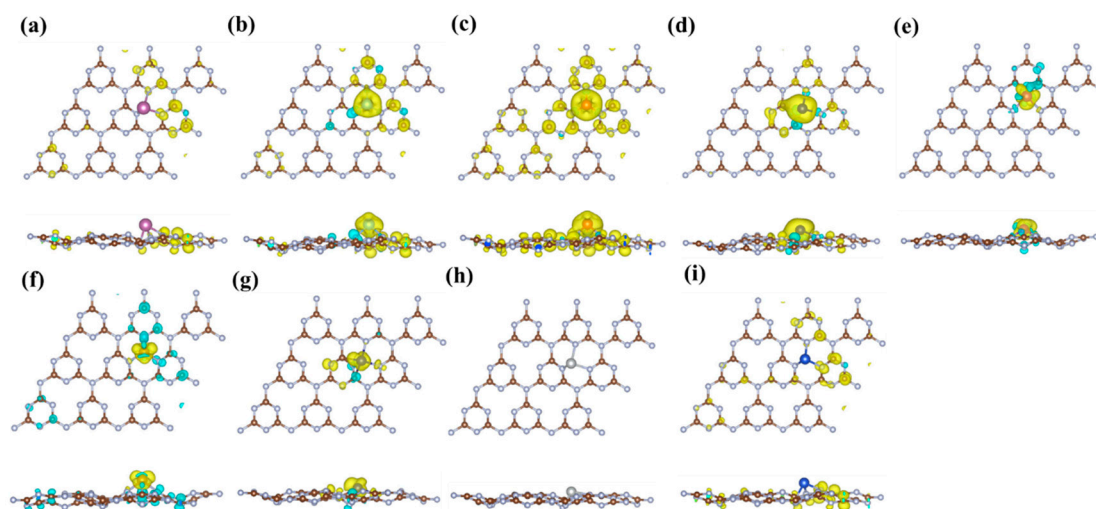
<sup>b</sup> College of physics and Electronic Engineering, Zhengzhou Normal University, Zhengzhou, Henan 450044, China

<sup>c</sup> School of Materials Science and Engineering, Henan Institute of Technology, Xinxiang, Henan 453000, China

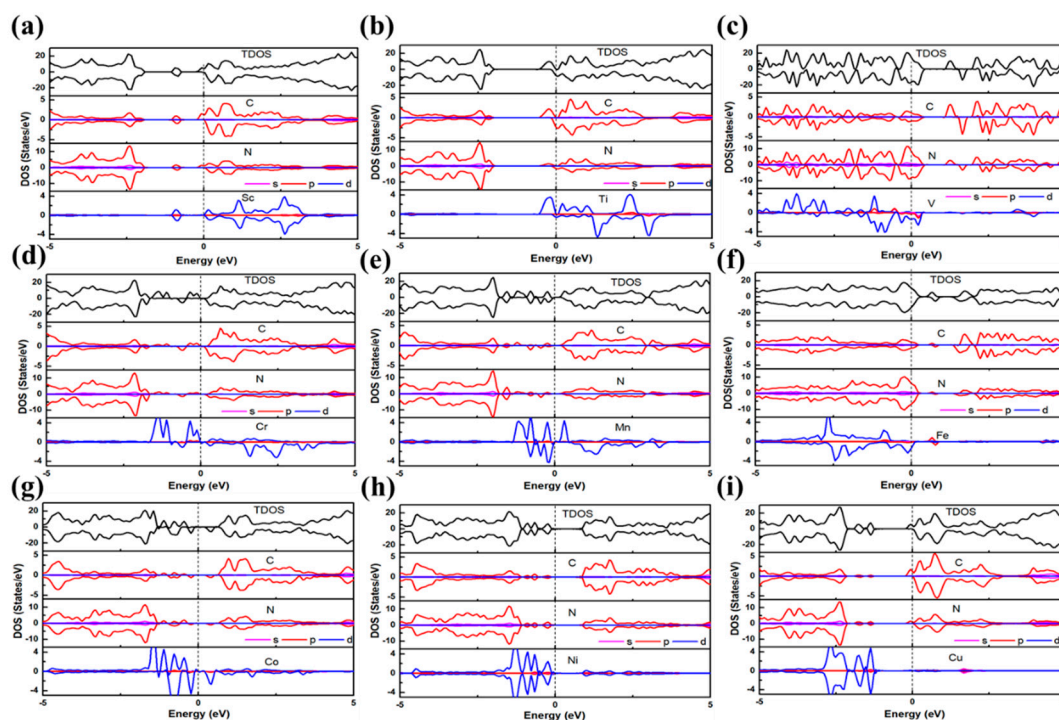
\* Correspondence: author, E-mail address: xqdai@htu.edu.cn (X. Dai), yntang2010@163.com (Y. Tang).



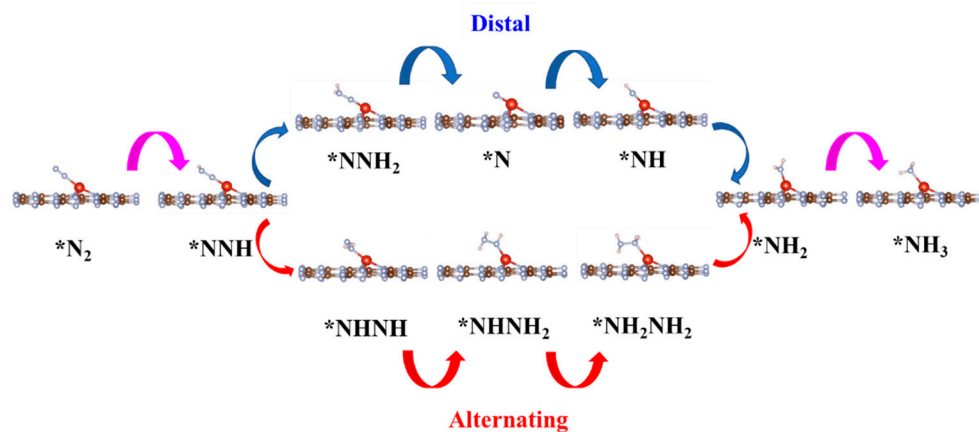
**Figure S1.** (a)-(h) Stable configurations of TM@g-C<sub>3</sub>N<sub>4</sub> (TM= Sc, Ti, V, Cr, Fe, Co, Ni, Cu).



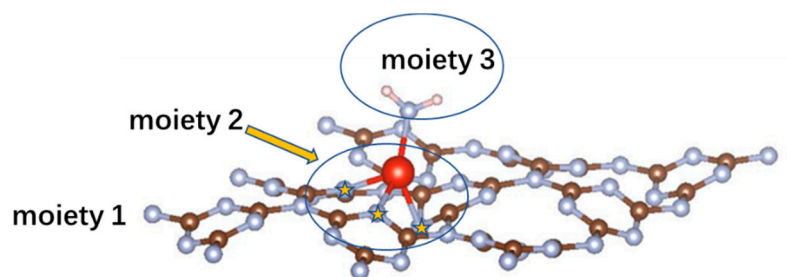
**Figure S2.** (a)-(i) Spin electron distributions of TM@g-C<sub>3</sub>N<sub>4</sub> (TM= Sc-Cu) with isosurface 0.004 e/Bohr<sup>3</sup>. Yellow and blue represent spin-up and spin-down states.



**Figure S3.** (a)–(i) DOS of TM@g-C<sub>3</sub>N<sub>4</sub> (TM= Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu). The Fermi level is set to zero.



**Figure S4.** Optimized adsorption structures of intermediate via the alternating and distal mechanisms.



**Figure S5.** Diagram of the moiety 1(g-C<sub>3</sub>N<sub>4</sub>), moiety 2 (V-3N) and moiety 3 (the adsorbed intermediate N<sub>3</sub>H<sub>7</sub>).