

Supporting Information for

Tuning Low-temperature CO oxidation Activities via N-doping on Graphene-Supported Three-Coordinated Nickel Single-Atom Catalysts

Tao Chen¹, Yujin Ji^{1*}, Yi-min Ding^{1,2}, Youyong Li^{1,3*}

¹ Institute of Functional Nano & Soft Materials (FUNSOM), Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Soochow University, Suzhou, Jiangsu 215123, China

² Yangtze Delta Region Institute (Huzhou), University of Electronic Science and Technology of China, Huzhou 313001, China

³ Macao Institute of Materials Science and Engineering, Macau University of Science and Technology, Taipa, Macau SAR 999078, China

*Corresponding author

E-mail: yjji@suda.edu.cn (Y. Ji); yyli@suda.edu.cn (Y. Li);

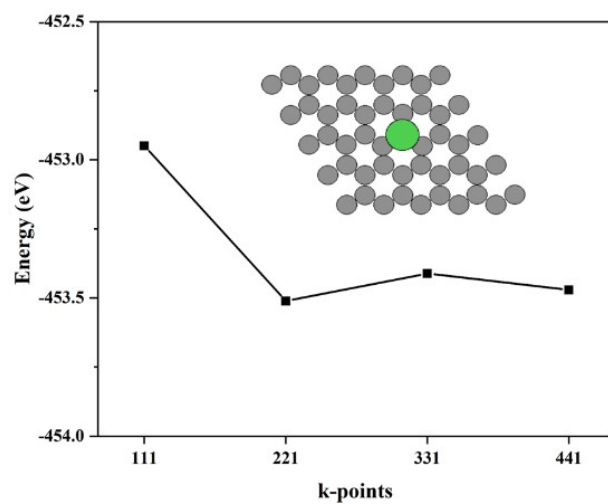


Figure S1. Total energies of Ni-N₀C₃ after geometric optimization for k-points converge test.

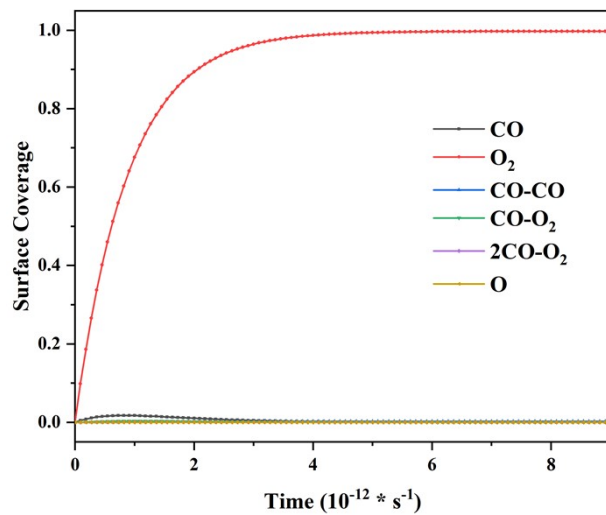


Figure S2. Surface coverages of reaction species numerically solved for Ni-N₁C₂ *versus* time interval for integrating the differential equations based on the organized microkinetic model.