

Electronic Supplementary Information

Copper on Carbon Materials: Stabilization by Nitrogen Doping

Dmitri A. Bulushev,^{*abc} Andrey L. Chuvilin,^{de} Vladimir I. Sobolev,^{ab} Svetlana G. Stolyarova,^b
Yury V. Shubin,^{bc} Igor P. Asanov,^{bc} Arcady V. Ishchenko,^{ac} Giacomo Magnani,^f Mauro Riccò,^f
Alexander V. Okotrub,^{bc} Lyubov G. Bulusheva^{*bc}

^a*Boriskov Institute of Catalysis, SB RAS, Novosibirsk, 630090, Russia*

^b*Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, 630090, Russia*

^c*Novosibirsk State University, Novosibirsk, 630090, Russia*

^d*CIC nanoGUNE Consolider, San Sebastian, 20018, Spain*

^e*IKERBASQUE, Basque Foundation for Science, Bilbao, 20013, Spain*

^f*Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma, 43124
Parma, Italy*

^{*}E-mail: dmitri.bulushev@catalysis.ru, bul@niic.nsc.ru

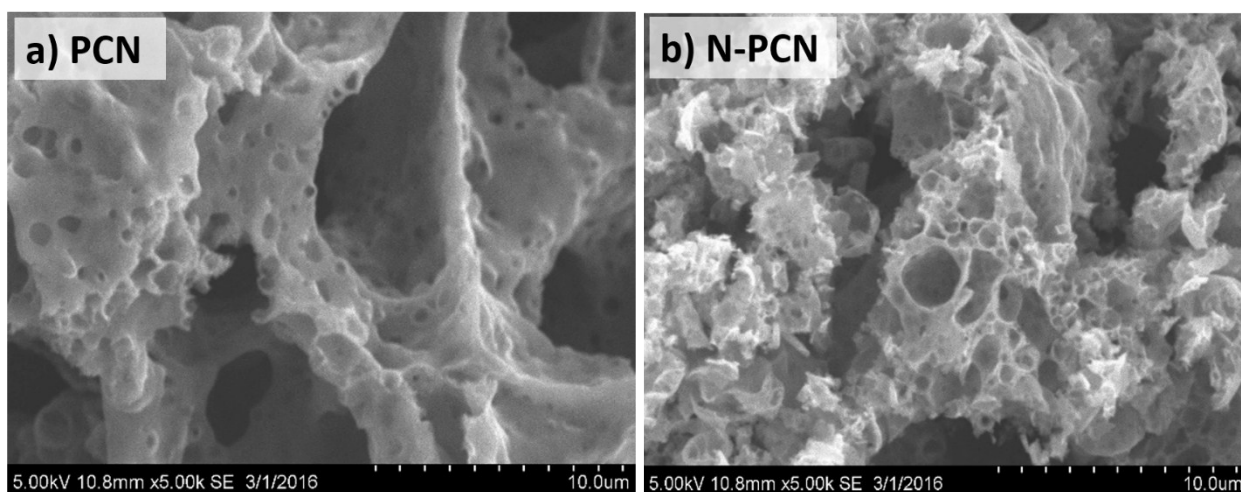


Figure S1. SEM images of the catalyst supports.

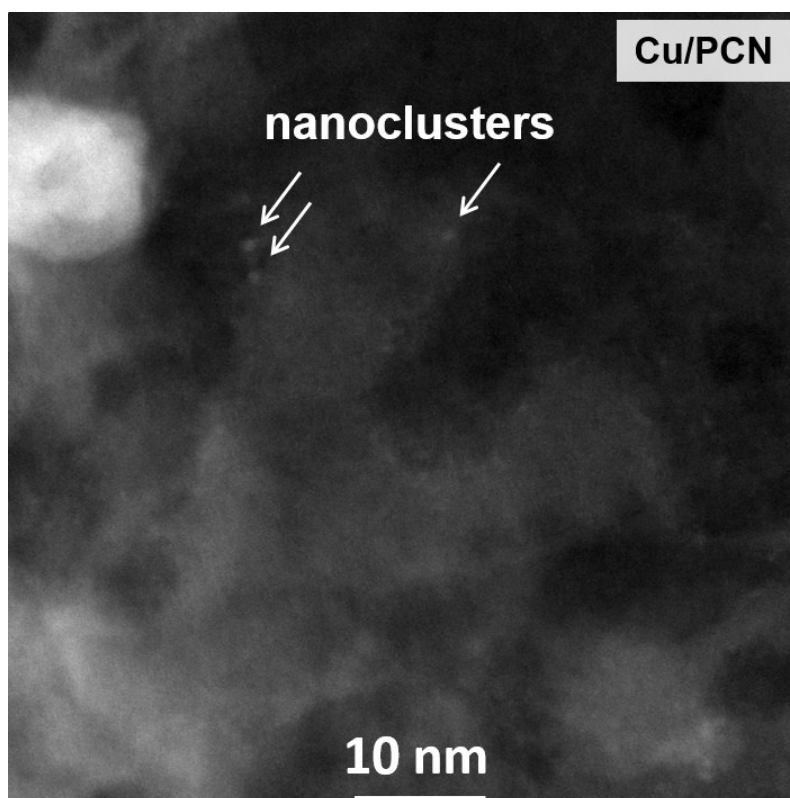


Figure S2. Atomic resolution HAADF/STEM image of the Cu/PCN catalyst after the reaction (Titan 60-300).

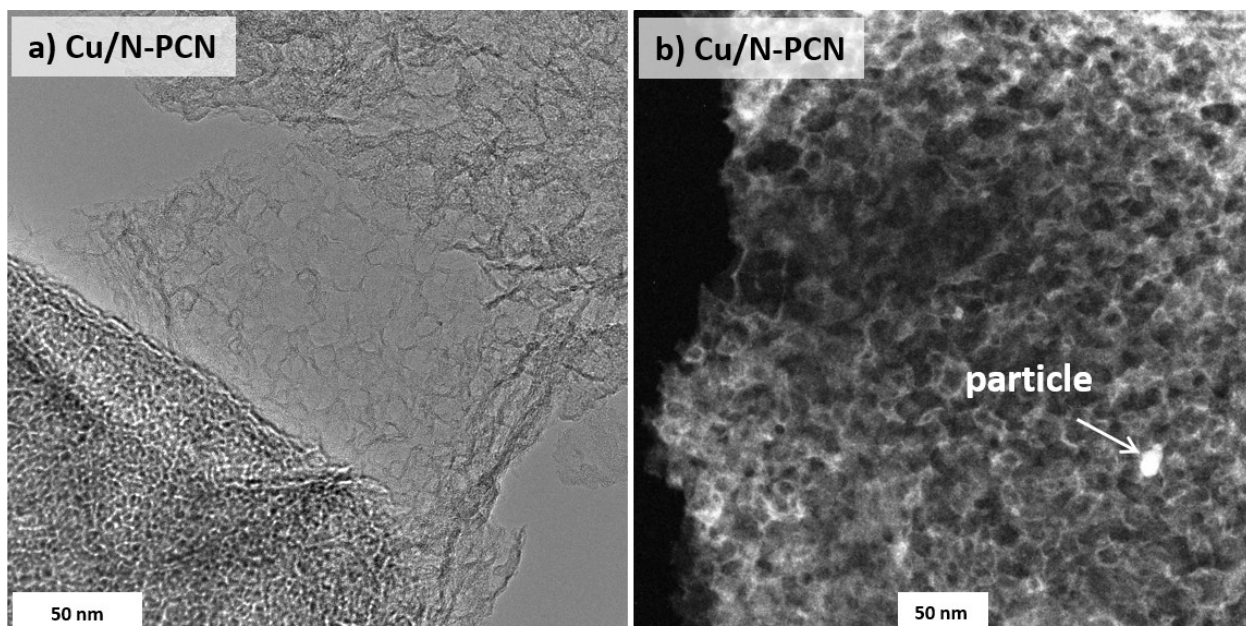


Figure S3. Low resolution a) TEM and b) HAADF/STEM images of the Cu/N-PCN catalyst after the reaction (Titan 60-300).

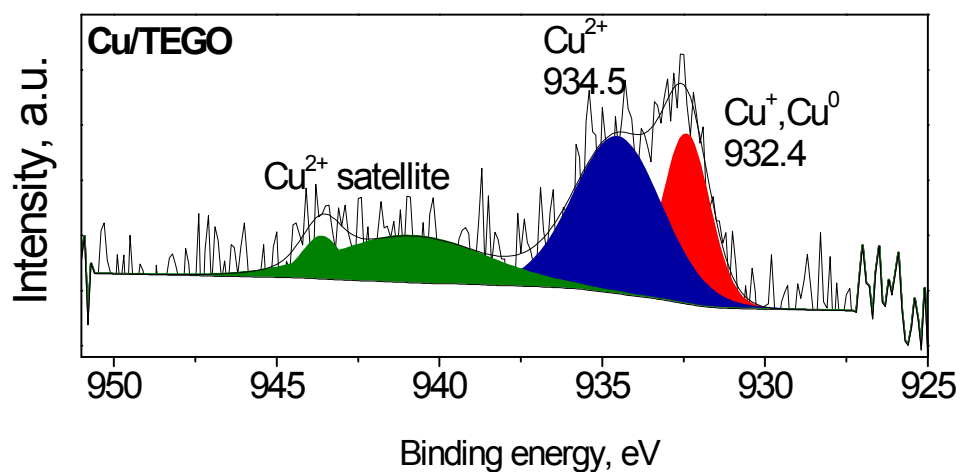


Figure S4. Cu $2p_{3/2}$ XPS spectra of the Cu/TEGO catalyst before the reaction.

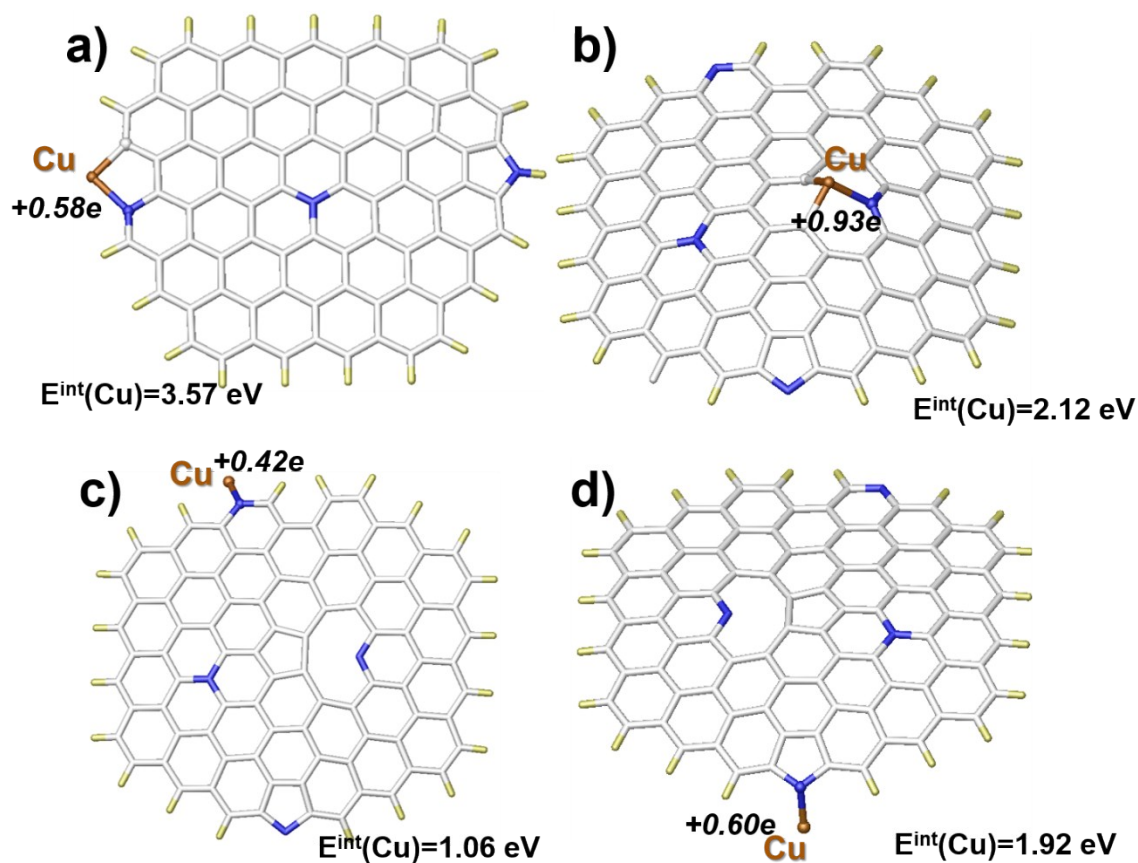


Figure S5. a),b),c),d) Models of binding of a Cu atom to the N-doped graphene fragments obtained after optimization at the PBE/LACVP level. White color indicates C, dark blue – N, yellow – H, and brown – Cu. The interaction energy of the Cu atom and NBO charge on it are indicated.

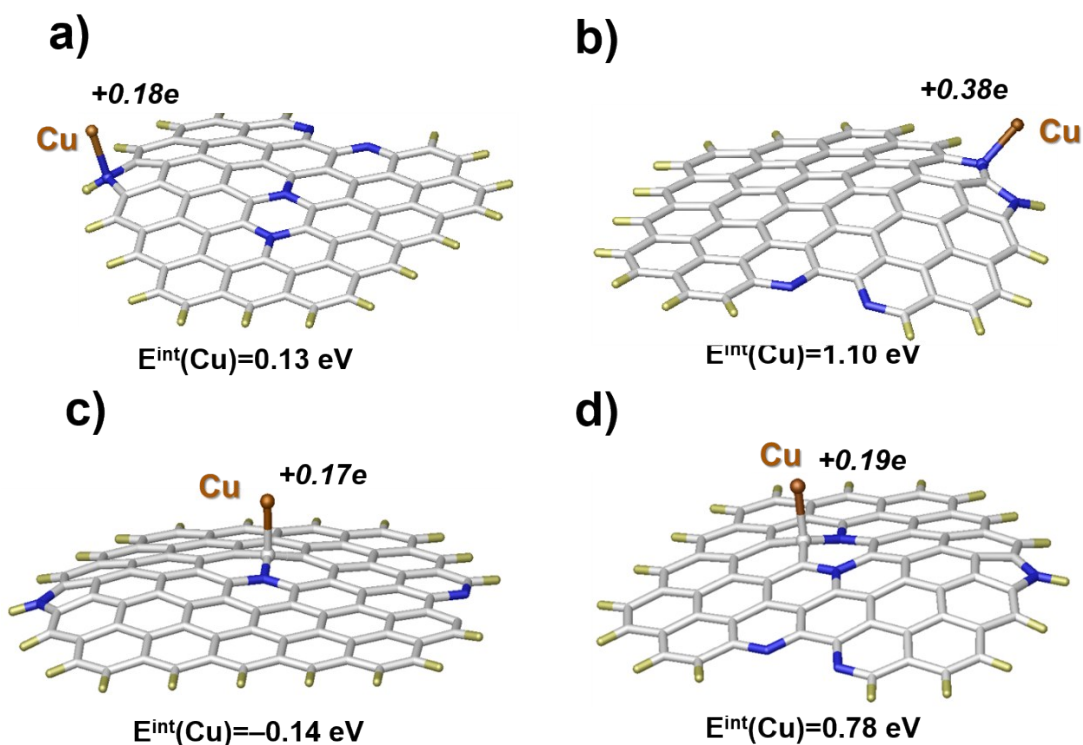


Figure S6. a),b),c),d) Models of binding of a Cu atom to the N-doped graphene fragments obtained after optimization at the PBE/LACVP level. White color indicates C, dark blue – N, yellow – H, and brown – Cu. The interaction energy of the Cu atom and NBO charge on it are indicated.

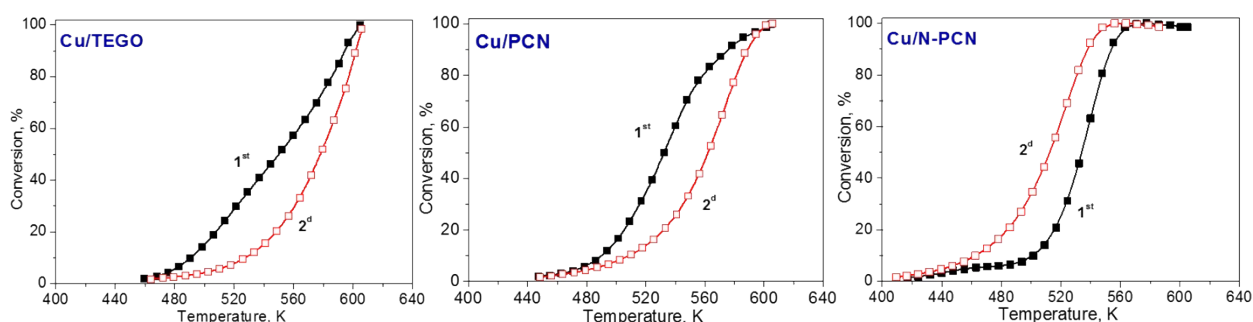


Figure S7. Formic acid conversion – temperature dependences for the Cu catalysts in the first and second heating cycles in formic acid (2 K min^{-1}).