Promoting effect of water on NH₃-SCR reaction over Cu-SAPO-34 catalyst: Transient

and permanent influences on Cu species

Yuyi Wan,^a Guangpeng Yang,^{a,b} Jinyao Xiang,^a Xiaoqiang Shen,^a Dafei, Yang,^a Yanrong Chen,^a Vladislav

Rac,^c Vesna Rakic ^c and Xuesen Du*^a

^a Key Laboratory of Low-grade Energy Utilization Technologies and Systems, School of Energy and Power Engineering, Chongqing University, Chongqing, 400044, China

^b Brook Byers Institute for Sustainable Systems and School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, GA 30332, United States

^c Faculty of Agriculture, Department of Chemistry, University of Belgrade, Nemanjina 6, 11080 Zemun, Serbia.



Fig. S1 NO conversion versus temperature data in standard SCR over Cu-SAPO-34 catalysts with Si/Al = 1/10 (a) Cu loading = 1.78 wt.% and (d) Si/Al = 1/4 Cu loading= 2.51 wt.% catalysts. Reactant feed contains 500 ppm of NO, 500 ppm of NH₃, 10% or 5% O₂, and 5% H₂O (if added) balanced with N₂ at a gas hourly space velocity (GHSV) of 300 000 h⁻¹



Fig. S2 Peak fitted results of NO conversions over Si/Al=1/10 Cu loading=1.16wt.% samples in the reaction feed with or without water.



Fig. S3 Structural illustration of $[Cu-O-Cu]^{2+}$ (a), $[Cu^{II}(OH)]^+$ (b), Z₂Cu-8MR (c), and Z₂Cu-6MR (d). Structures of of $[Cu-O-Cu]^{2+}$ (e), $[Cu^{II}(OH)]^+$ (f), Z₂Cu-8MR (g), and Z₂Cu-6MR (h) with additional $[Cu^{II}(OH)]^+$ nearby.