Supporting Information

Shape-Controlled CeO_2 Nanoparticles: Stability and Activity in the Catalyzed HCl Oxidation Reaction

Chenwei Li[a,b], Yu Sun[a], Igor Djerdj[c], Pascal Voepel[b], Carl-Christian Sack[b], Tobias Weller[b], Joachim Sann[b], Rüdiger Ellinghaus[b], Yanglong Guo[a,*], Bernd M. Smarsly[b,*], Herbert Over[b,*]

a) Key Laboratory for Advanced Materials, Research Institute of Industrial Catalysis, School of Chemistry and Molecular Engineering, East China University of Science and Technology, Shanghai 200237, PR China
b) Physikalisch-Chemisches Institut, Justus-Liebig-University, Heinrich-Buff-Ring 17, 35392 Giessen, Germany
c) Department of Chemistry, J. J. Strossmayer University of Osijek, Ulica cara Hadrijana 8/a, HR-31000 Osijek , Croatia

* *Corresponding authors:* E-mail:
herbert.over@phys.chemie.uni-giessen.de
Bernd.Smarsly@phys.Chemie.uni-giessen.de
ylguo@ecust.edu.cn

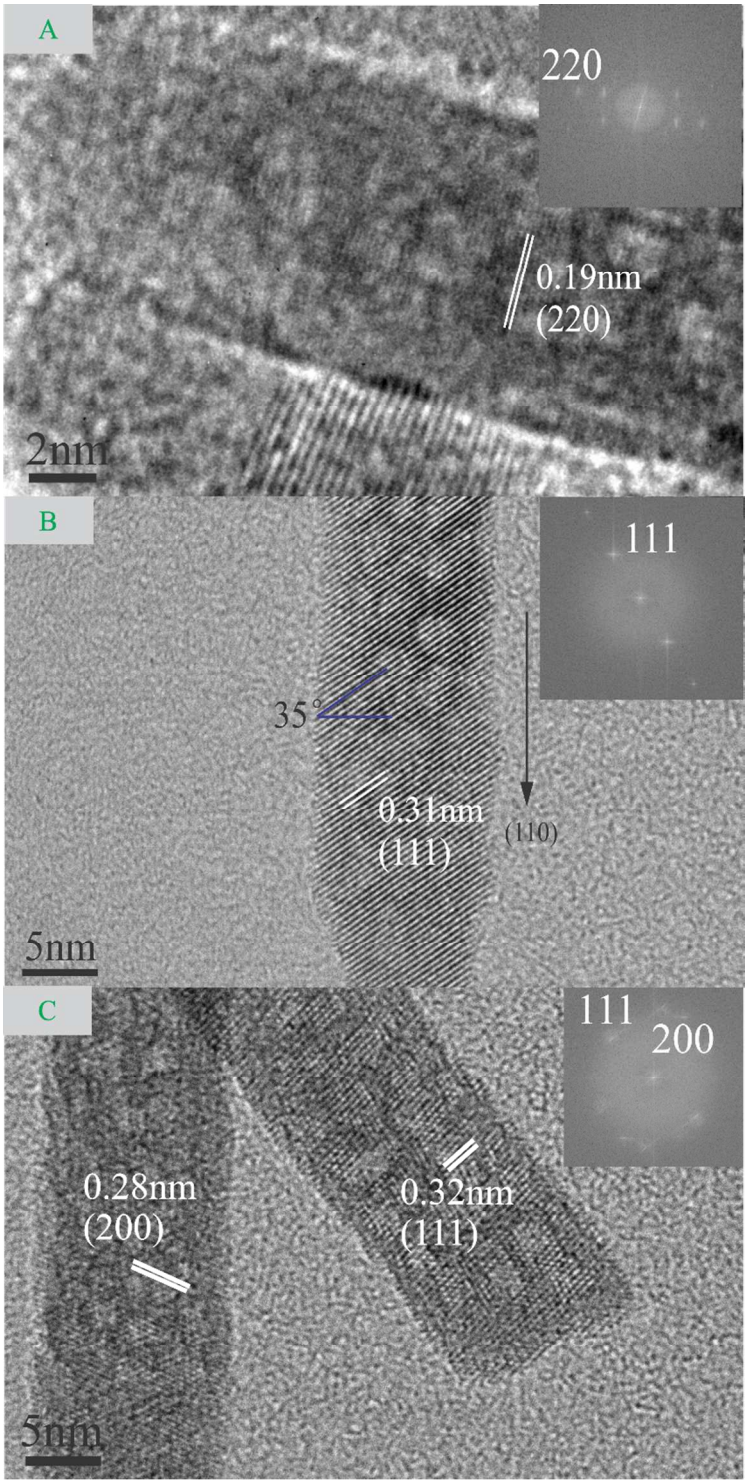

Figure S1: High-resolution TEM images of the as-prepared shape controlled CeO_2 nanorods. Inset: Fast Fourier Transformation (FFT) pattern of each particle

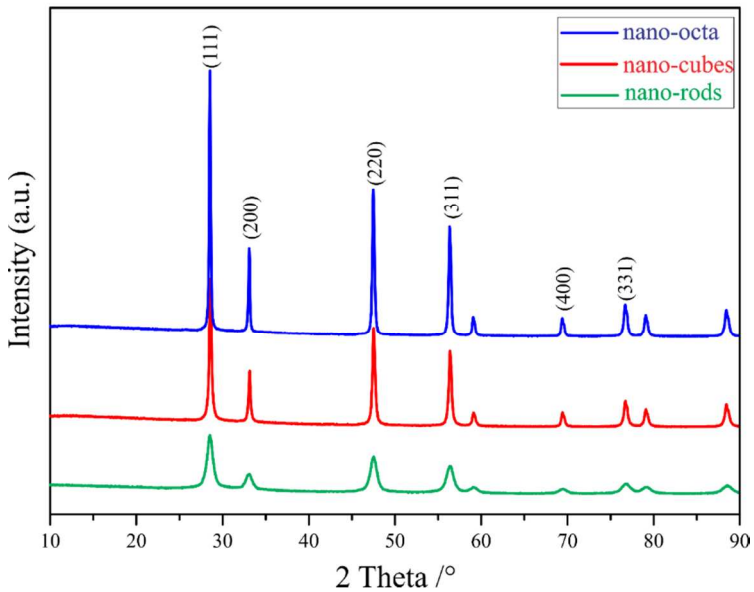

Figure S2: XRD scans of the as-prepared shape controlled CeO_2 particles: (blue) octahedrons; (red) cubes; (green) rods.

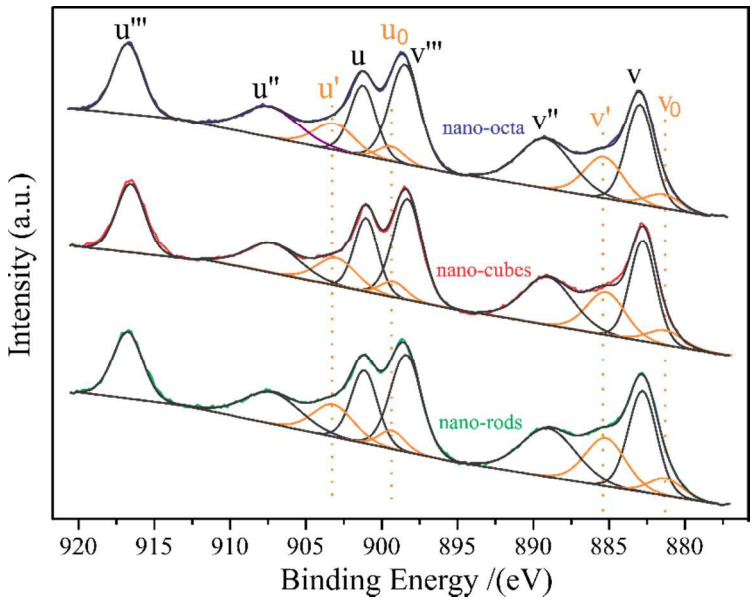

Figure S3: XPS spectra of Ce3d of as-prepared shaped-controlled CeO_2 nanoparticle and their deconvolution into Ce^{3+} and Ce^{4+} related emissions (octahedrons, cubes and rods).

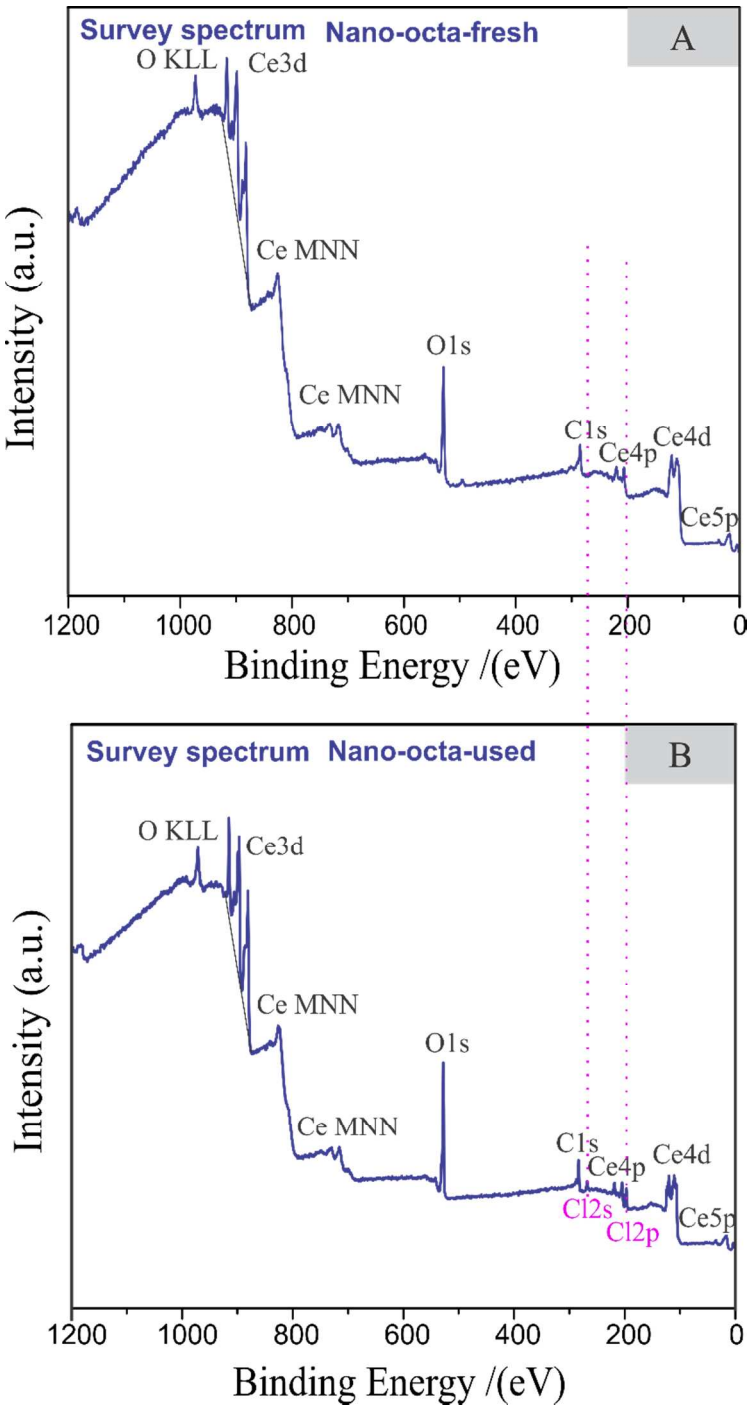

Figure S4: XPS spectra of survey: **A)** as-prepared CeO_2 nano-octahedron; **B)** CeO_2 nano-octahedron after Deacon reaction of harsh condition.

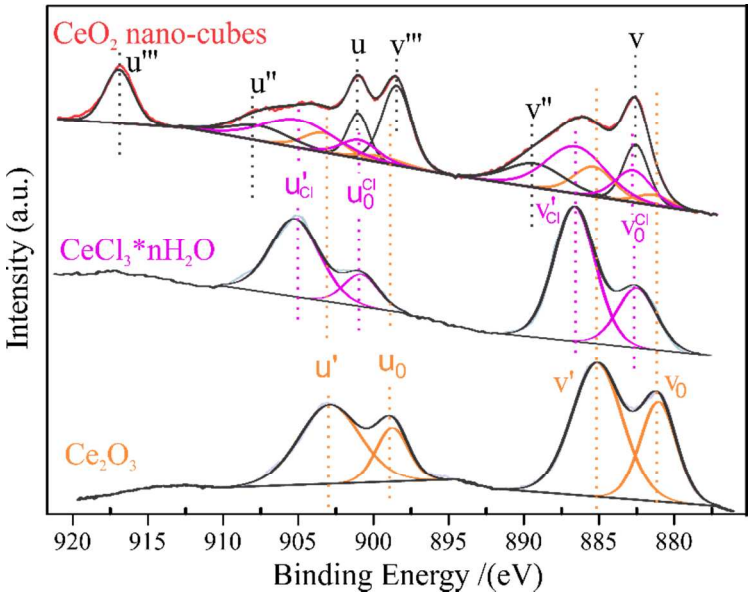

Figure S5: XPS spectra of Ce3d of CeO_2 nano-cubes after Deacon reaction under harsh condition. XP reference spectra of pure $CeCl_3$*nH_2O and pure Ce_2O_3 are utilized for the curve fitting of the CeO_2 nano-cube spectrum. Details of Ce_2O_3 reference spectra measurement: Air oxidized Ce foil was evaporated in UHV by an e-beam evaporator on a Ru(0001) single crystal surface up to a film thickness of 3 ML. The XPS measurement was conducted in the same UHV chamber using MgK_α radiation and a Leybold EA 200 analyzer.

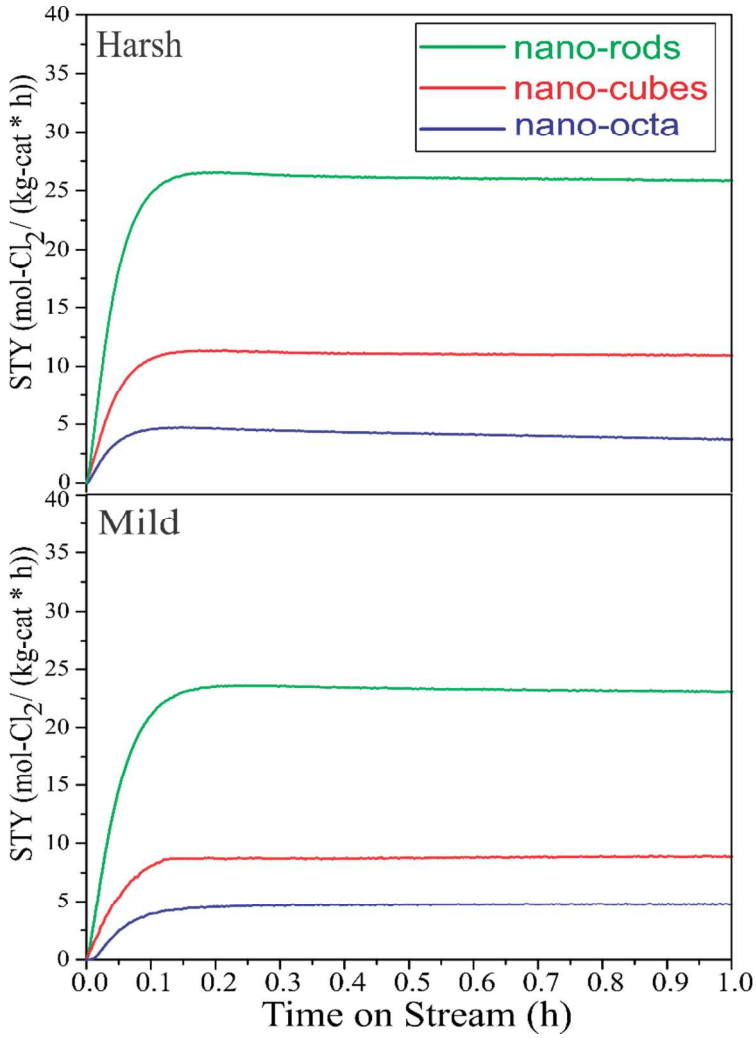

Figure S6: Space time yield (STY) of molecular chlorine in the HCl oxidation reaction using shape-controlled CeO_2 nanoparticle (octahedrons, cubes and rods). The temperature during the reaction was T = 430 °C. a) harsh reaction conditions: Ar:HCl:O_2=6:2:2 and b) mild reaction conditions: Ar:HCl:O_2=7:1:2 and a flow rate of 15 sccm.

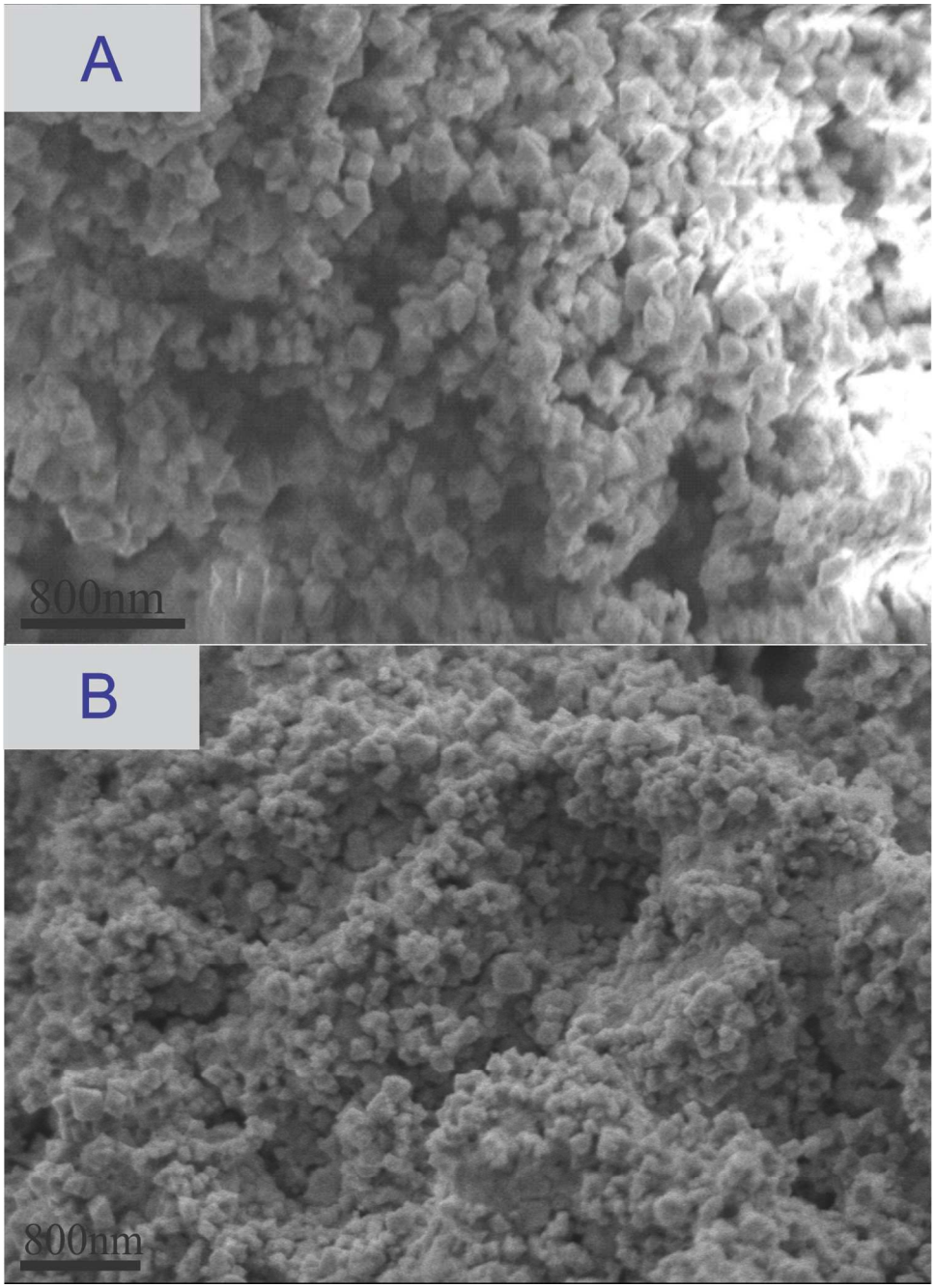

Figure S7: SEM images of the CeO_2 nano-octahedrons after the Deacon reaction under harsh condition