

## **Anomalous catalytic and antibacterial activity confirmed by molecular docking analysis of silver and polyacrylic acid doped CeO<sub>2</sub> nanostructures**

Muhammad Ikram<sup>a</sup>, Rizwan Karim<sup>b</sup>, Ali Haider<sup>c</sup>, Anum Shahzadi<sup>d</sup>, Mohammed M Algaradah<sup>e</sup>, Anwar Ul-Hamid<sup>f\*</sup>, Walid Nabgan<sup>g</sup>, Ahmed M. Fouda<sup>h</sup>, Salamat Ali<sup>b</sup>

<sup>a</sup>Solar Cell Applications Research Lab, Department of Physics, Government College University Lahore, Lahore, 54000, Punjab, Pakistan

<sup>b</sup>Department of Physics, Riphah Institute of Computing and Applied Sciences (RICAS), Riphah International University, 14 Ali Road, Lahore, Pakistan

<sup>c</sup>Department of Clinical Sciences, Faculty of Veterinary and Animal Sciences, Muhammad Nawaz Shareef University of Agriculture, Multan, 66000, Pakistan

<sup>d</sup>Faculty of Pharmacy, The University of Lahore, 54000, Pakistan

<sup>e</sup>Chemistry Department, King Khalid Military Academy, Riyadh 11495, Saudi Arabia

<sup>f</sup>Core Research Facilities, Research Institute, King Fahd University of Petroleum & Minerals, Dhahran, 31261, Saudi Arabia

<sup>g</sup>Departament d'Enginyeria Química, Universitat Rovira i Virgili, Av Països Catalans 26, 43007, Tarragona, Spain.

<sup>h</sup>Chemistry Department, Faculty of Science, King Khalid University, Abha 61413, Saudi Arabia

\*Corresponding authors' emails: <sup>a</sup>[dr.muhammadikram@gcu.edu.pk](mailto:dr.muhammadikram@gcu.edu.pk), <sup>g</sup>[wnabgan@gmail.com](mailto:wnabgan@gmail.com), <sup>f</sup>[anwar@kfupm.edu.sa](mailto:anwar@kfupm.edu.sa)

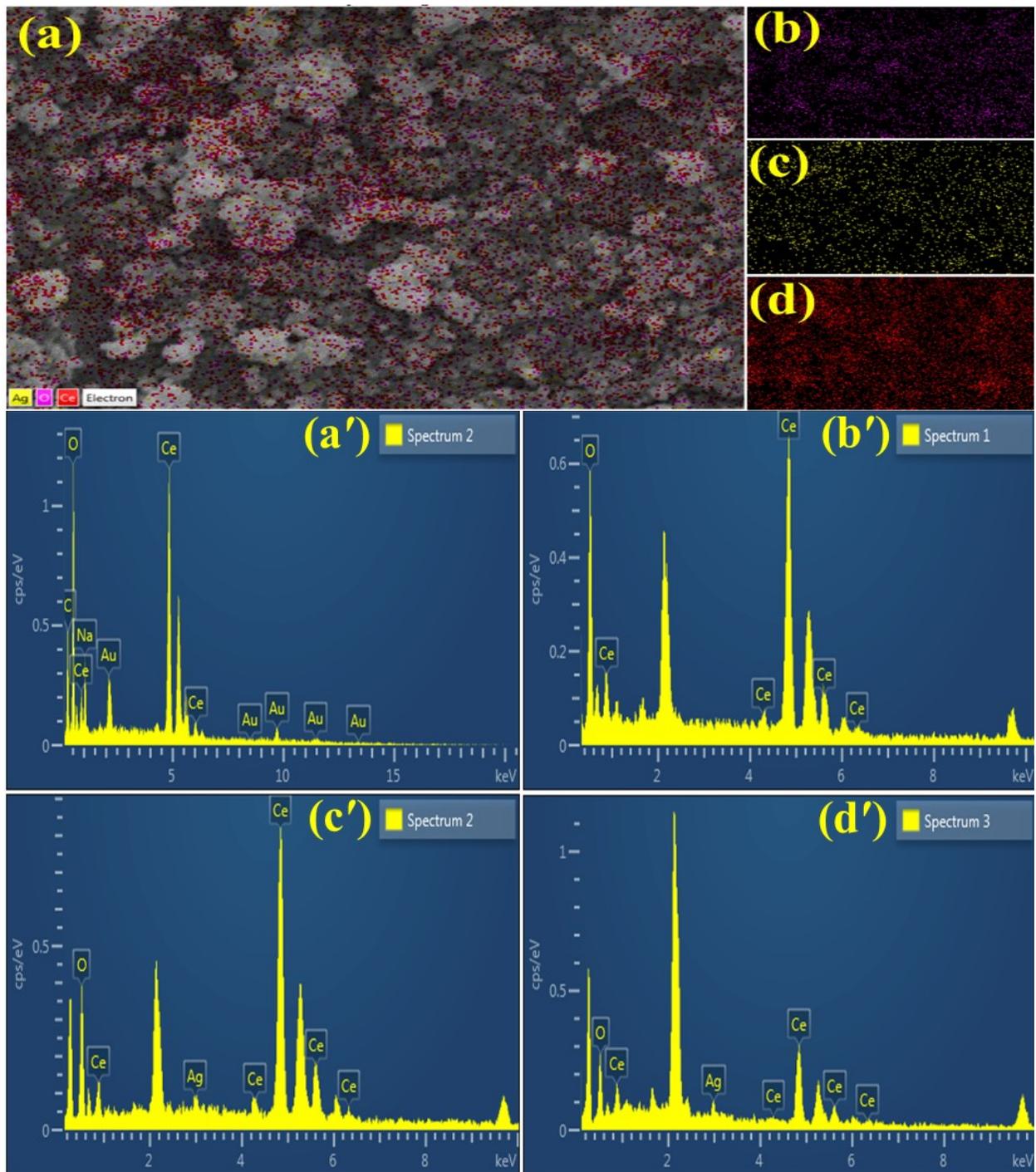


Figure S1: (a-d) Mapping of (0.03) Ag/PAA doped CeO<sub>2</sub> and (a'-d') EDS spectra of pure and (0.01, 0.03) Ag/PAA doped CeO<sub>2</sub>

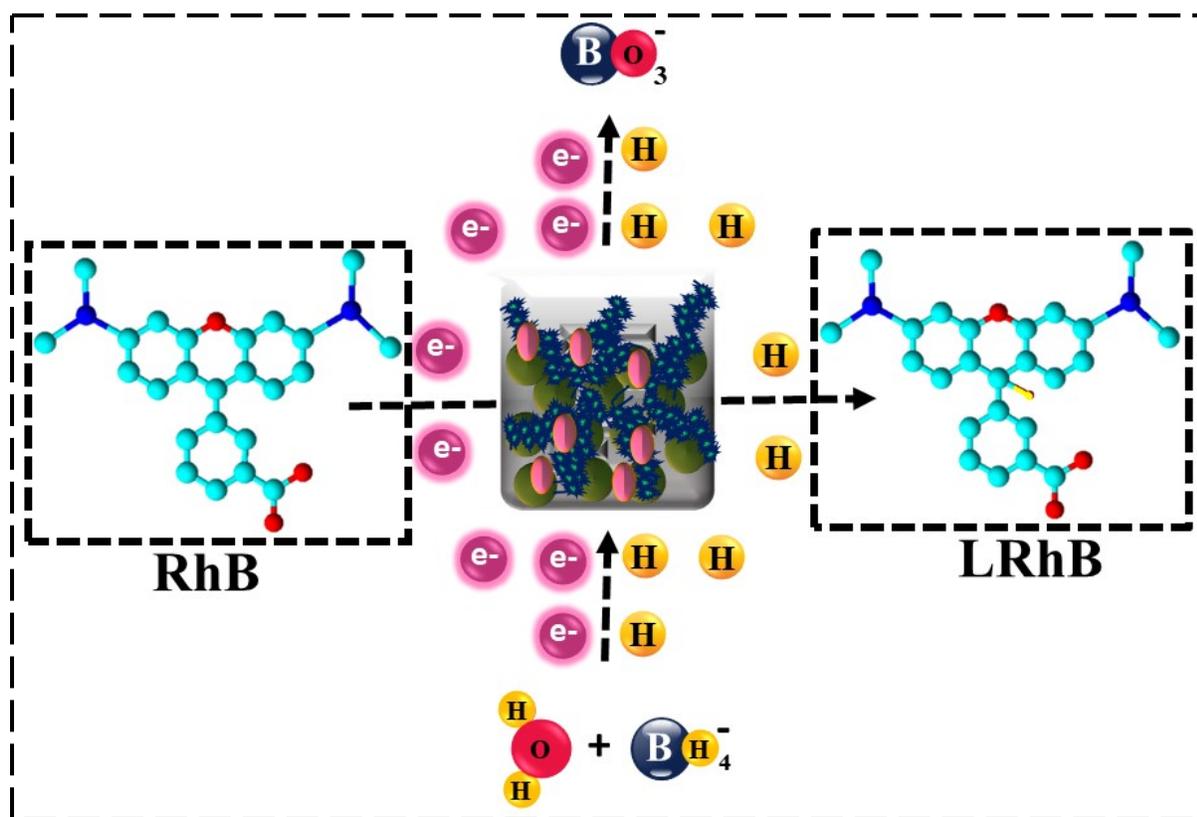


Figure S2: Catalysis mechanism of Ag/PAA doped CeO<sub>2</sub>

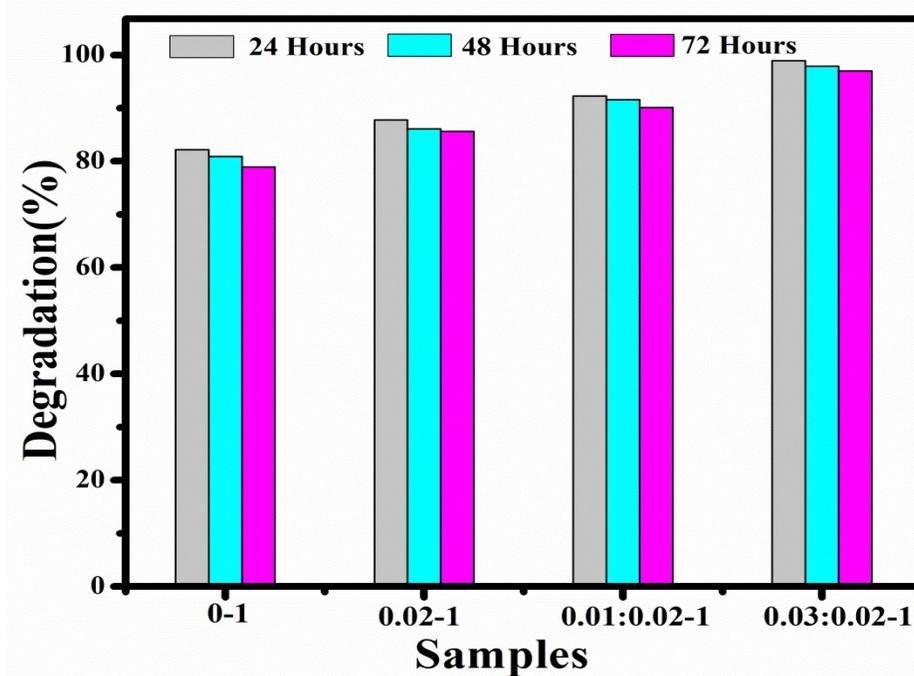


Figure S3: Stability tests of  $\text{CeO}_2$  and (0.01, 0.02) Ag/PAA doped  $\text{CeO}_2$  in acidic medium

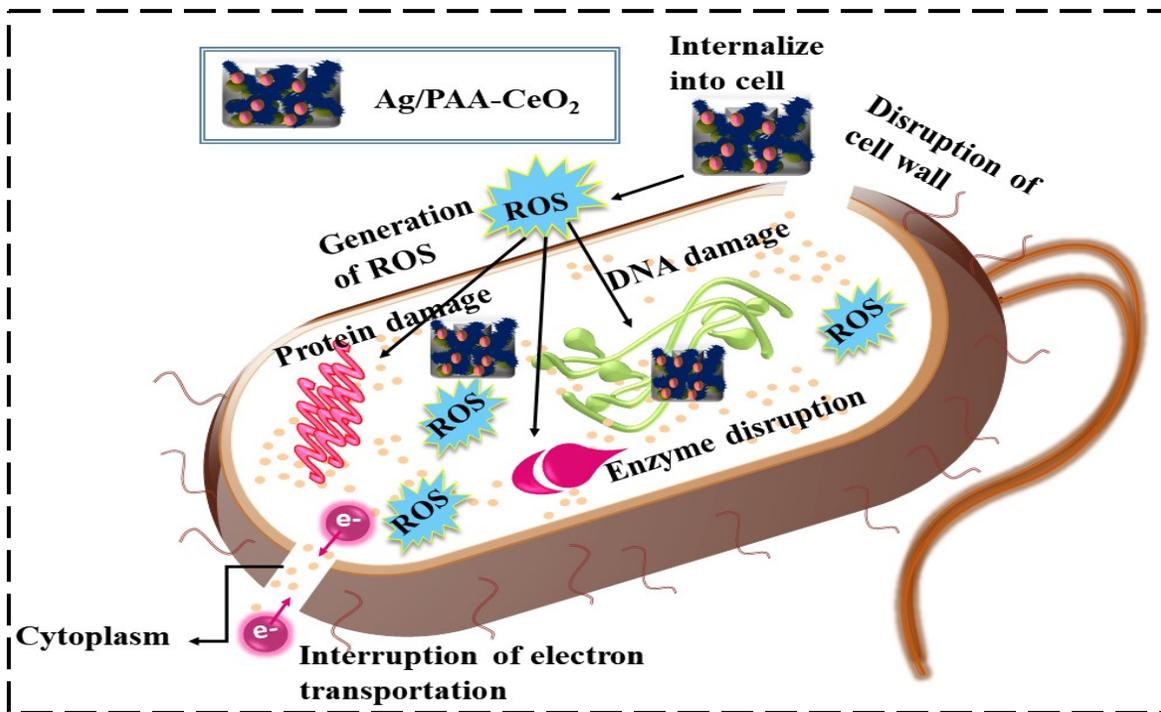


Figure S4: Antibacterial activity of Ag/PAA doped  $\text{CeO}_2$

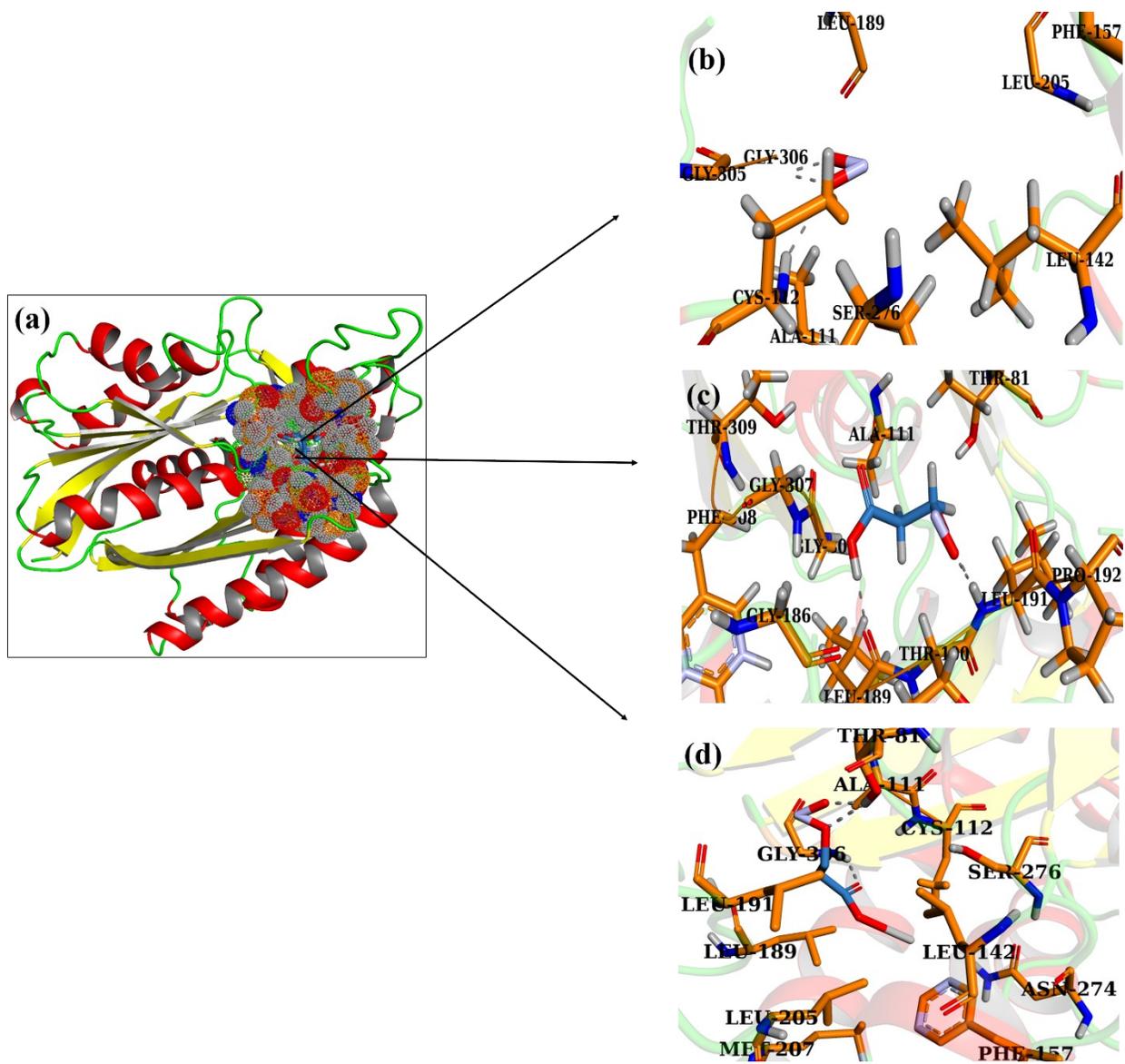


Figure S5: 3D representation of superimposed ligands inside the active site (a) and binding interaction of NSs inside the active site of FabH<sub>E. coli</sub> (b) CeO<sub>2</sub>, (c) PAA-CeO<sub>2</sub>, and (d) Ag/PAA-CeO<sub>2</sub>.

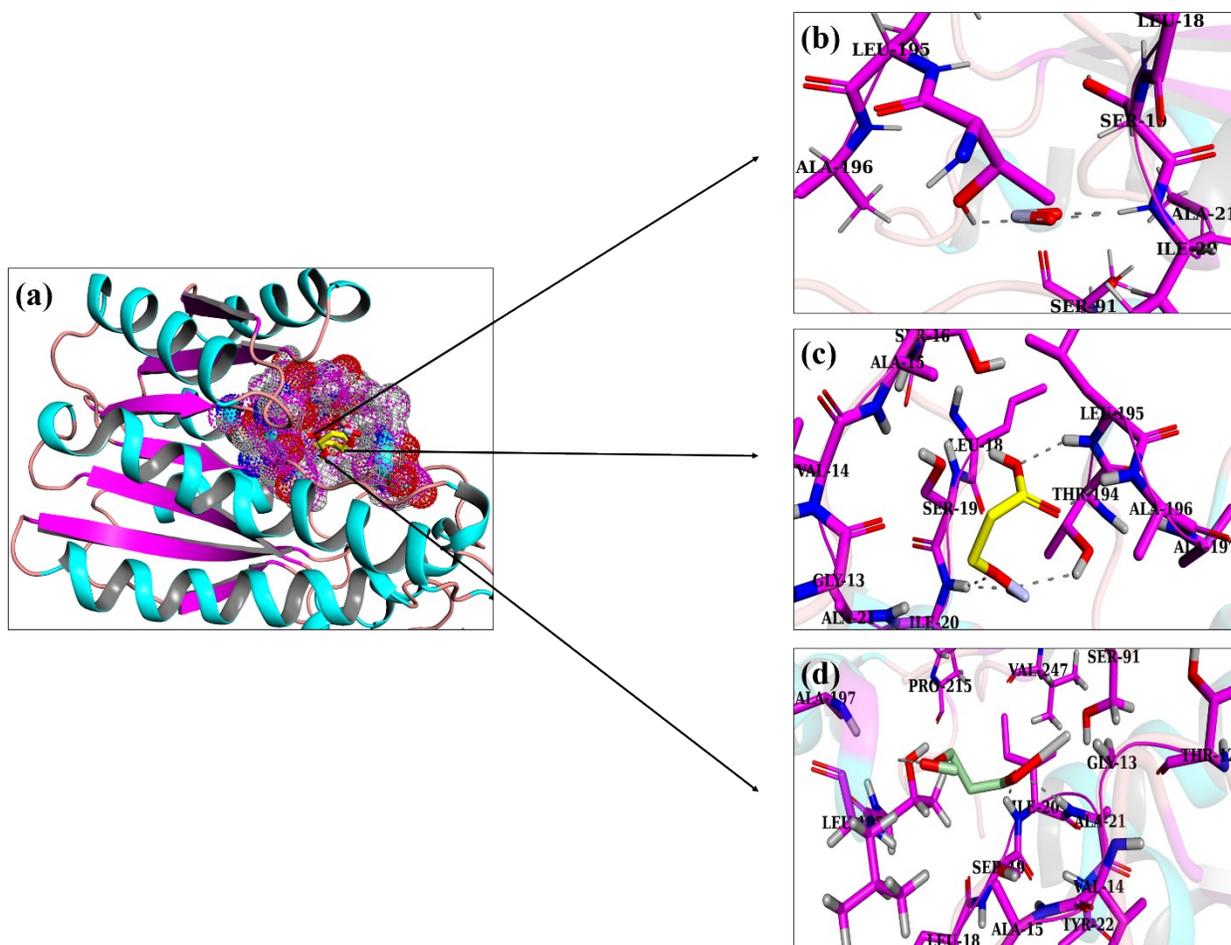


Figure S6: 3D representation of superimposed ligands inside the active site (a) and binding interaction of NSs inside the active site of FabI<sub>E. coli</sub> (b) CeO<sub>2</sub>, (c) PAA-CeO<sub>2</sub>, and (d) Ag/ PAA-CeO<sub>2</sub>.