Supplementary Material

Investigating the catalytic and antimicrobial properties of ternary cesium/polyethylene glycol-SrO supported by molecular docking and DFT analysis

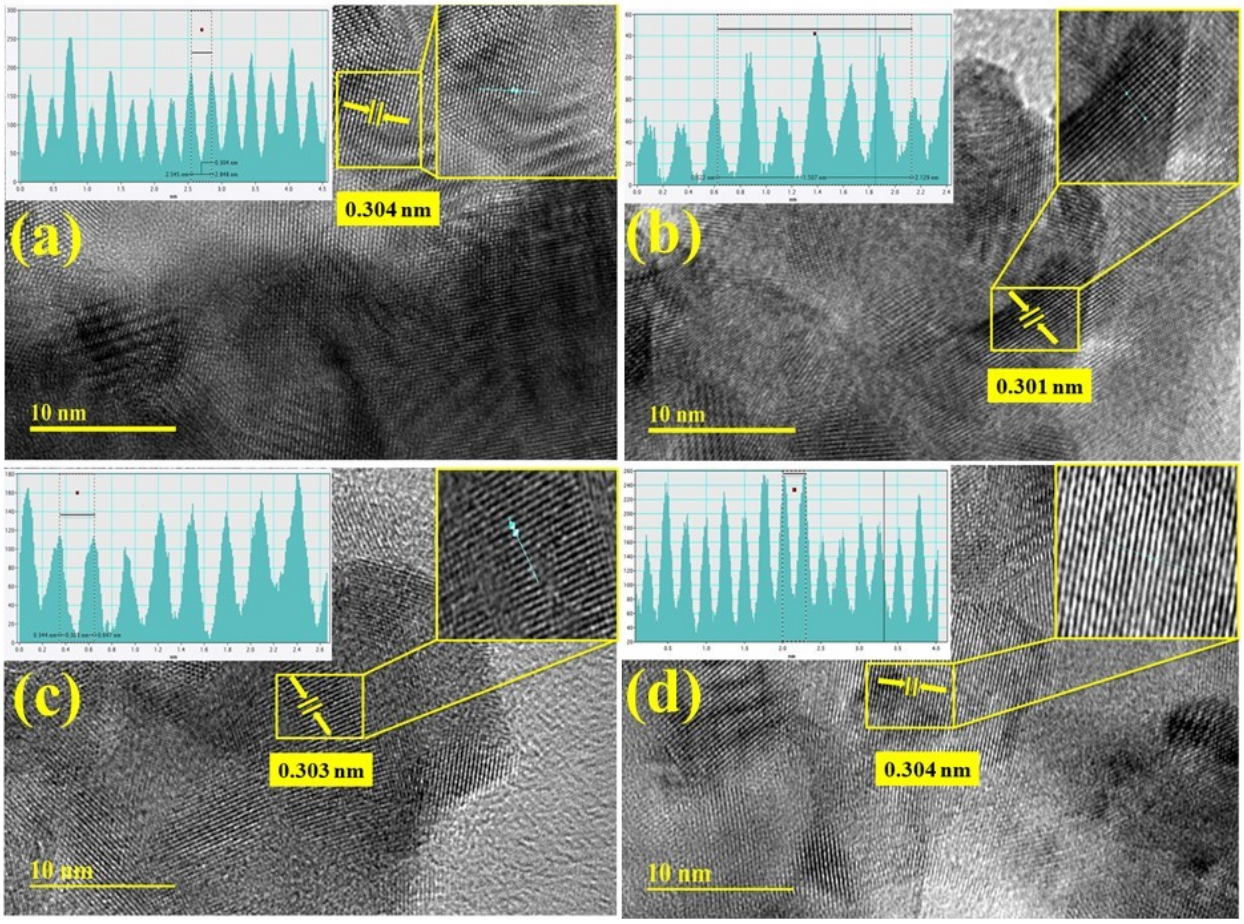

Fig. S1. HRTEM d-spacing of (a), SrO (b), PEG-SrO (c, d) (2 and 4 wt. %) Cs/PEG-SrO

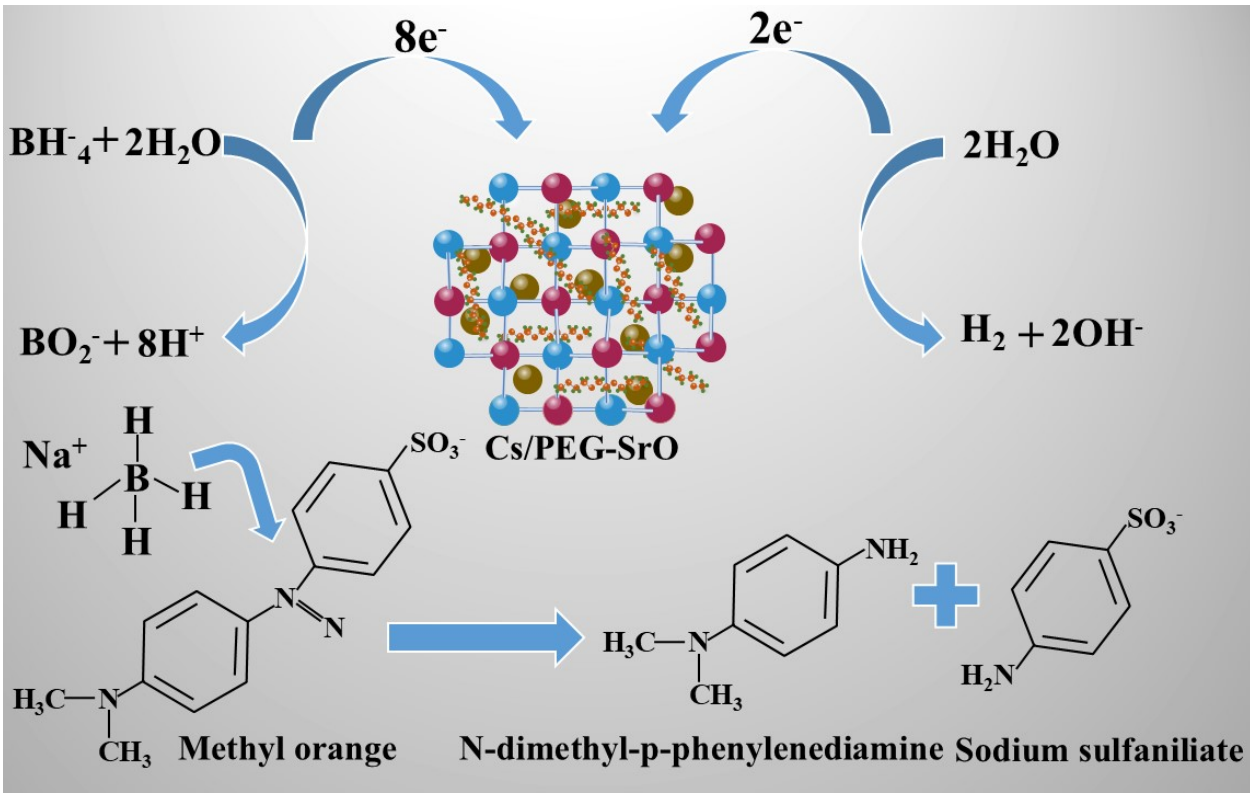

Fig. S2. Schematic diagram of catalytic dye degradation in the presence of pristine and doped SrO

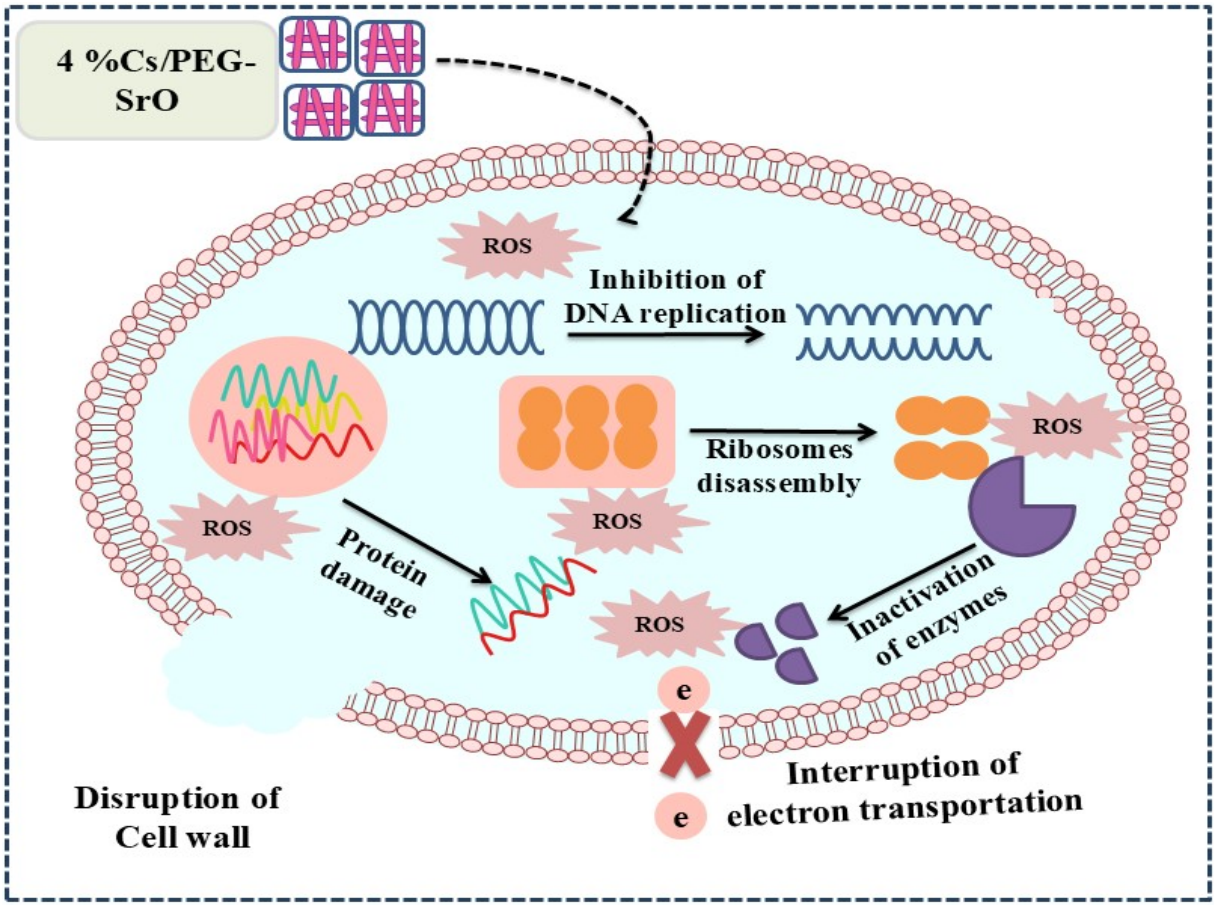

Fig. S3. Antibacterial behavior of SrO, and doped SrO

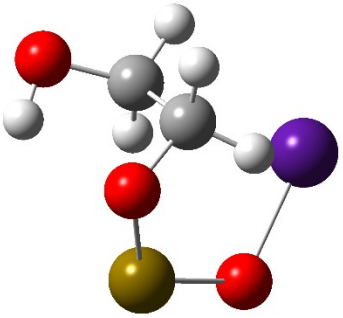

Fig. S4. Molecular Structure of Cs/PEG-SrO

Table S1. DFT calculation (Quantum chemical descriptors) of specified ligand.

Ligand	Cs/PEG-SrO (Gas)	Cs/PEG-SrO (Aqueous)
Dipole moment (Debye)	3.3390	2.9779
HOMO (a.u.)	-0.11628	-0.09379
LUMO (a.u.)	0.05757	0.01852
Energy Gap (ΔE_{Gap})	1.598 eV	2.049 eV
Ionization Potential (eV)	3.164	2.552
Electron affinity (eV)	1.568	0.504
Electronegativity χ (eV)	2.366	1.528
Electrochemical potential μ (eV)	-2.366	-1.528
Hardness η (eV)	0.798	1.024
Softness S (eV^{-1})	1.253	0.977
Electrophilicity ω (eV)	3.506	1.141

Table S2. Coordinates of Cs/PEG-SrO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-6.592900	3.855800	-2.576000
2	6	0	-5.803300	3.964800	-1.352900
3	6	0	6.637000	3.372800	-0.181000
4	8	0	-7.120900	2.085700	-0.579500

5	38	0	-5.360000 1.189200 -0.602200
6	8	0	-3.770000 1.830700 0.436900
7	55	0	-3.648100 3.925000 0.758400
8	1	0	-6.667600 2.894600 -2.605100
9	1	0	-5.540400 4.999600 -1.097100
10	1	0	-4.842000 3.434600 -1.480800
11	1	0	-7.495600 4.018800 0.015100
12	1	0	-6.085900 3.230400 0.755700