

## Supplementary Information

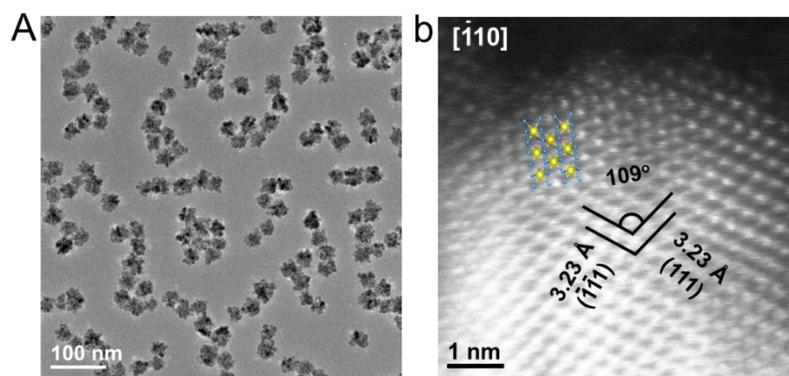
### **Synergistic effect between polyvinyl pyrrolidone and oxygen vacancies on improving oxidase-mimetic activity of flower-like CeO<sub>2</sub> Nanozymes**

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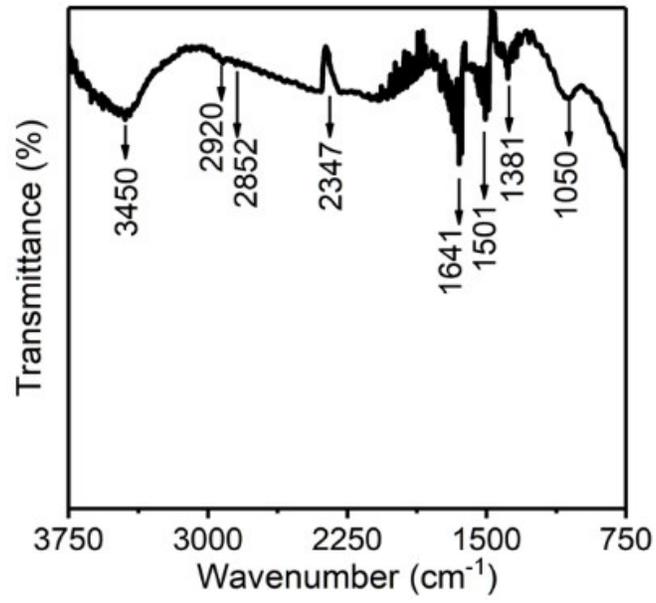
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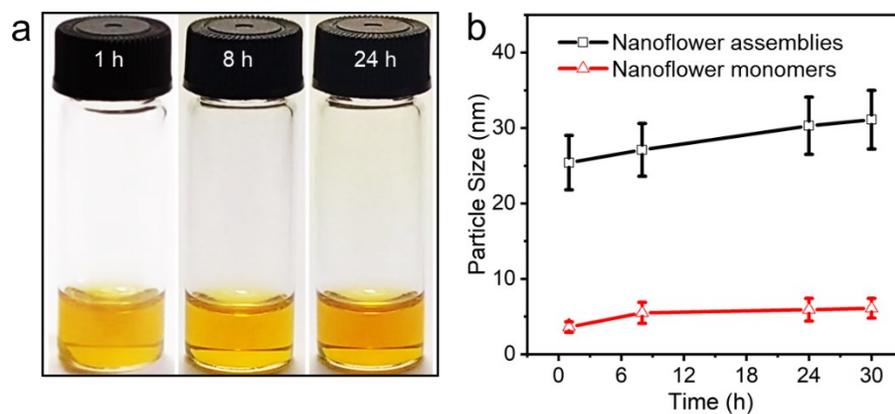
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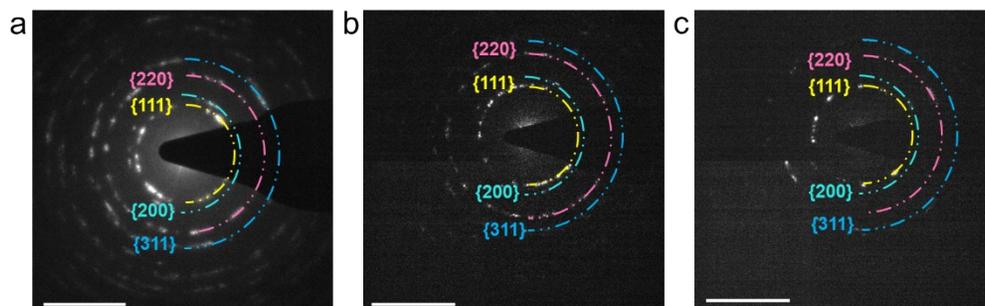
**Fig. S1** (a) TEM image, (b) High-resolution STEM image of the one representative CeO<sub>2</sub> nanoflower.



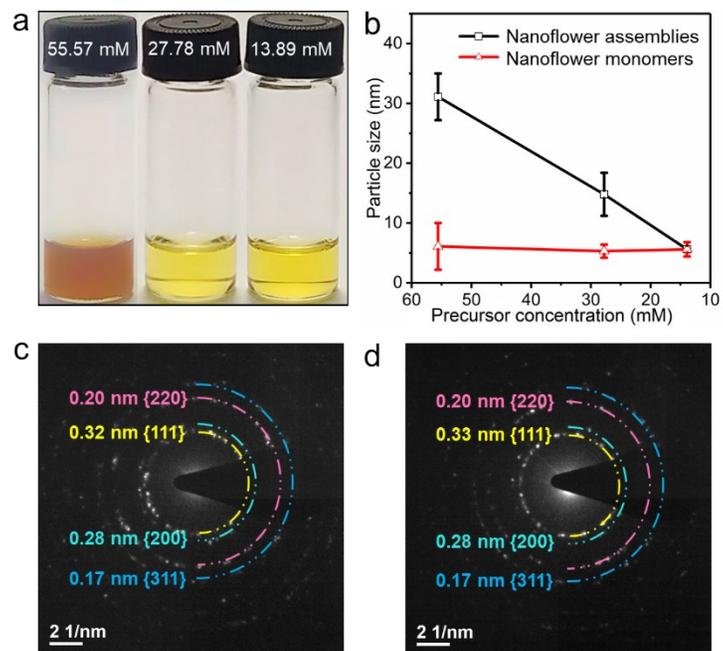
**Fig. S2** FTIR spectrum of CeO<sub>2</sub> nanoflowers.



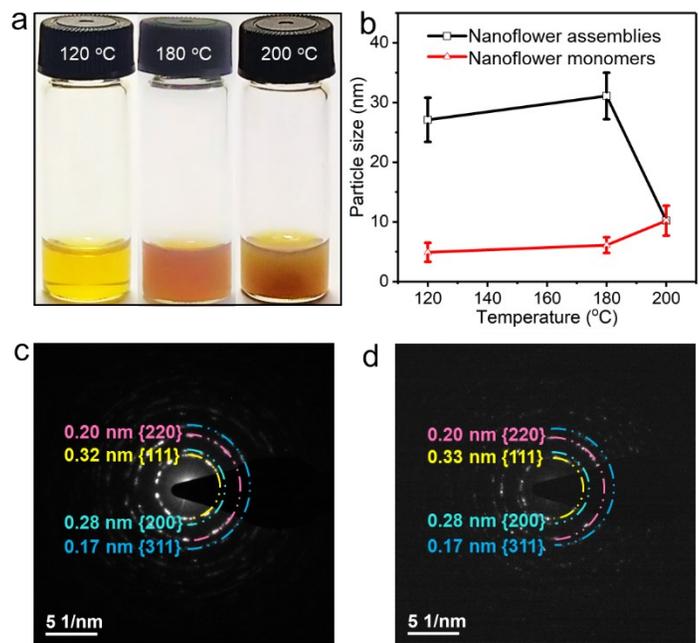
**Fig. S3** (a) Optical images and (b) average-size evolutions of nanoflower assemblies and monomers obtained at different solvothermal durations.



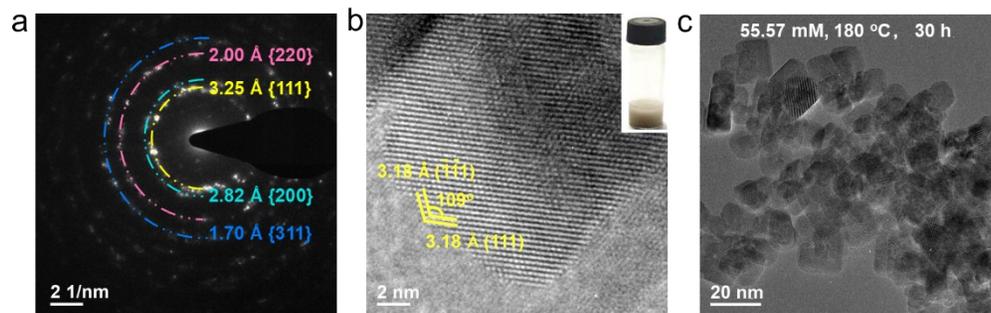
**Fig. S4** SAED patterns of CeO<sub>2</sub> nanoflowers obtained at different solvothermal durations: (a) 1 h, (b) 8 h, and (c) 24 h. Scale bar: 5 1/nm.



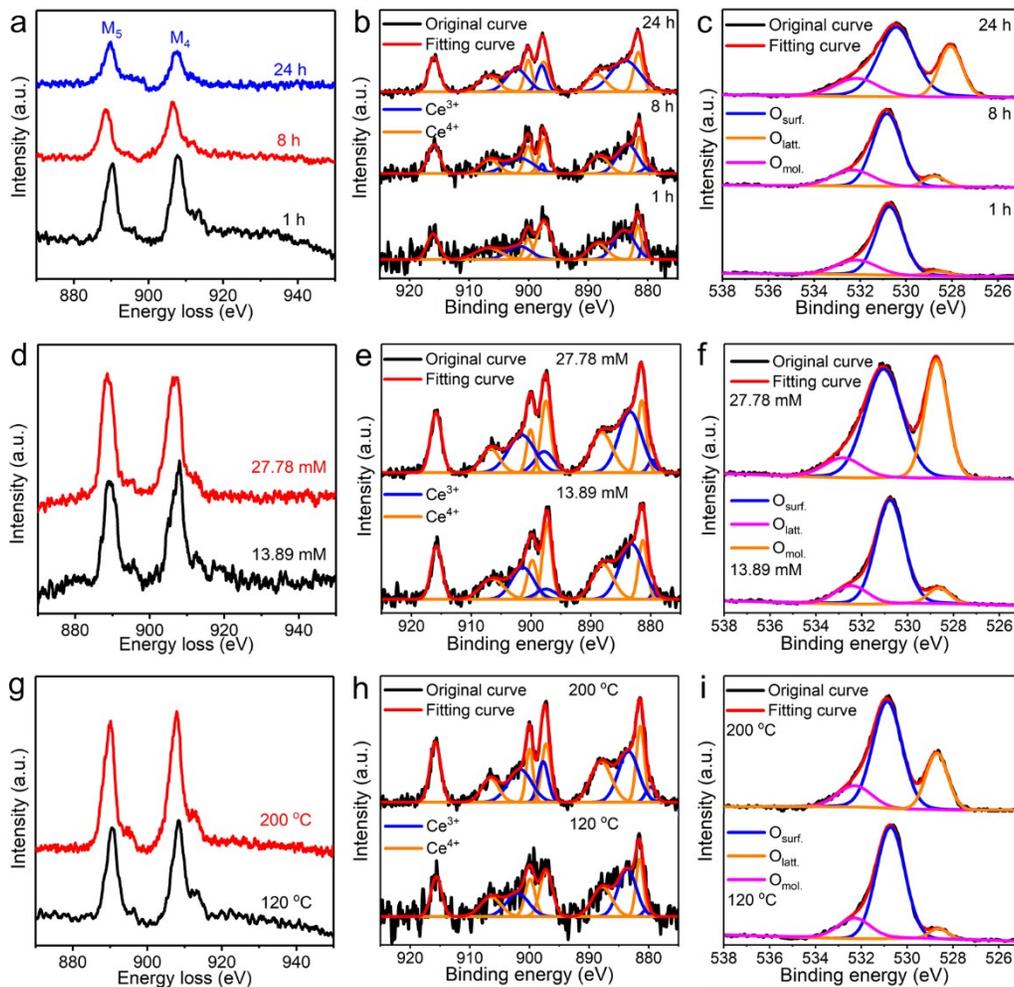
**Fig. S5** (a) Optical images, (b) average-size evolutions, and (c-d) SAED patterns of CeO<sub>2</sub> nanoflowers obtained from different precursor concentrations: (c) 27.78 mM, (d) 13.89 mM.



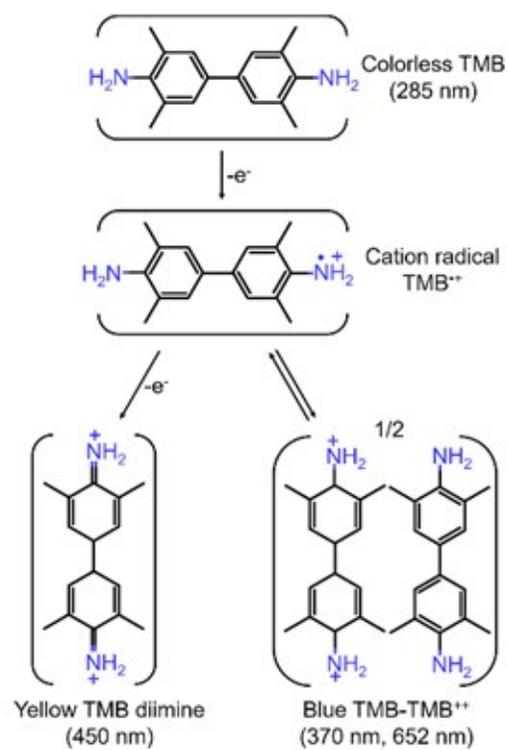
**Fig. S6** (a) Optical images, (b) average-size evolutions, and (c–d) SAED patterns of CeO<sub>2</sub> nanoflowers obtained at different reaction temperatures: (c) 120 °C, (d) 200 °C.



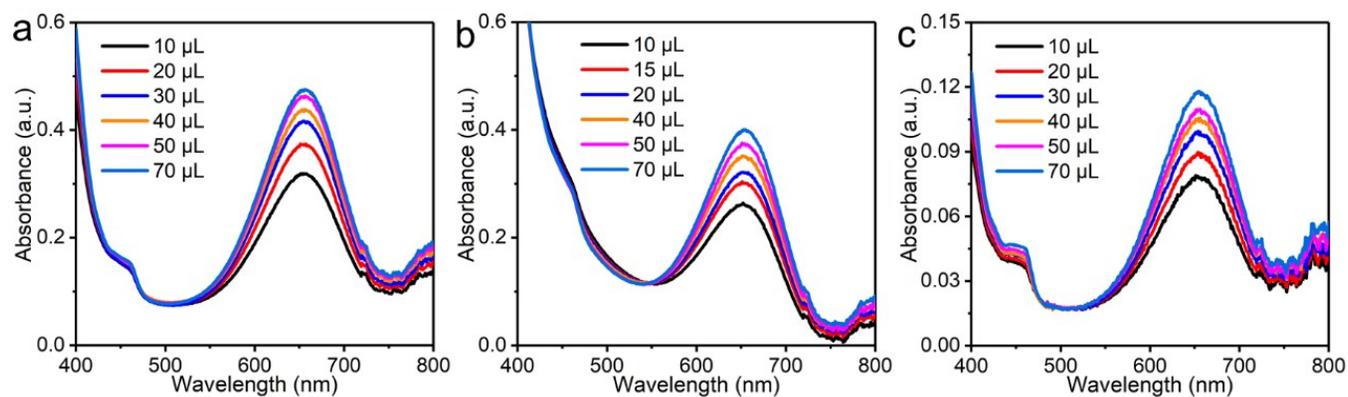
**Fig. S7** (a) SAED pattern, and (b–c) HRTEM images of CeO<sub>2</sub> nanocubes obtained in the absence of PVP. Inset in (b) is the corresponding optical image.



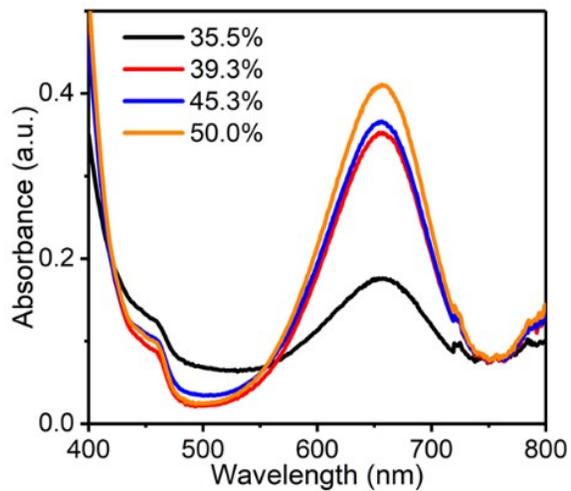
**Fig. S8** (a, d and g) EELS, and (b–c, e–f, and h–i) XPS spectra of a CeO<sub>2</sub> nanoflowers obtained at different conditions: (a–c) at different reaction durations, (d–f) from different precursor concentrations, (g–h) at different solvothermal temperatures. Specifically, EELS for Ce-M<sub>5,4</sub> edge, and XPS for Ce 3*d* and O 1*s*.



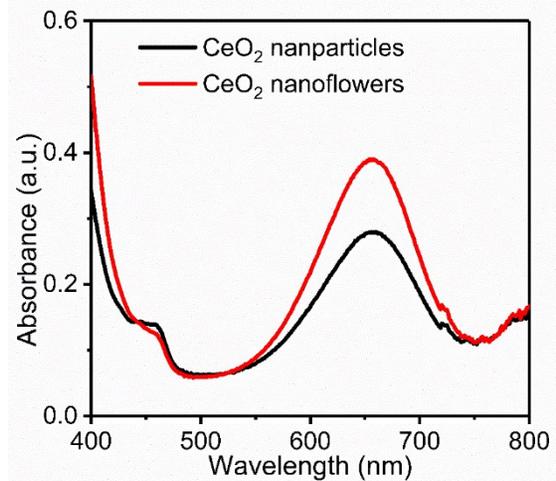
**Fig. S9** Oxidation process of TMB.



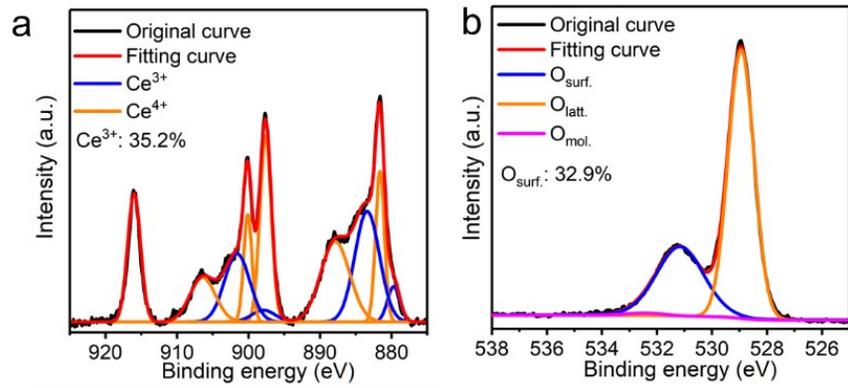
**Fig. S10** TMB-dependent UV-vis absorption spectra of the mixture containing (a) 2 μmol of 31.1-nm CeO<sub>2</sub> nanoflowers, (b) 0.5 μmol of 5.6-nm CeO<sub>2</sub> nanocubes, and (c) 2 μmol of 10.1-nm CeO<sub>2</sub> nanocubes. The concentration of the used TMB is 10 mM.



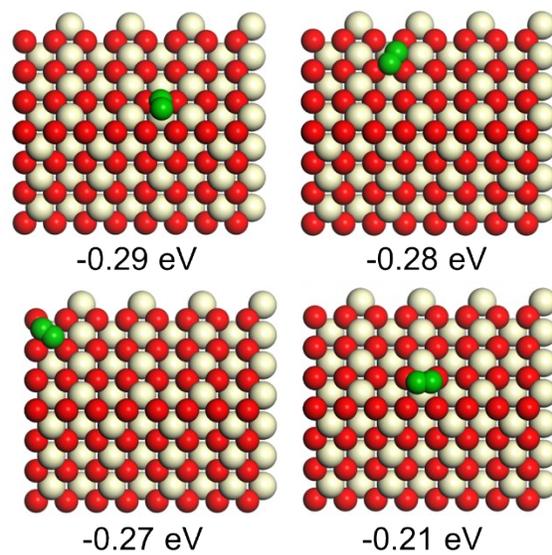
**Fig. S11** UV-vis absorption spectra of the TMB solutions catalyzed by CeO<sub>2</sub> nanoflowers with different Ce(III) percentages.



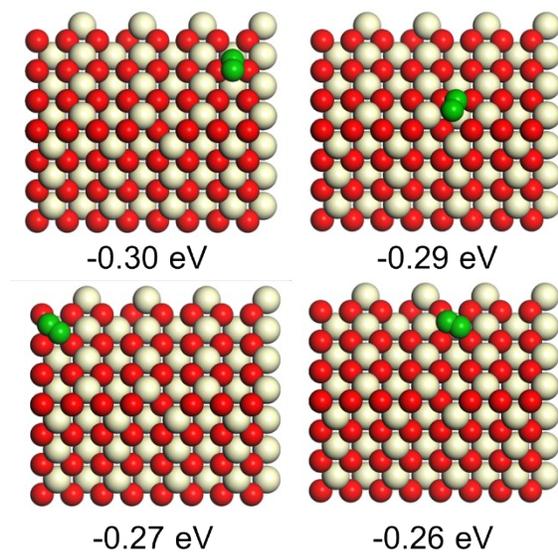
**Fig. S12** UV-vis spectra of TMB solution catalyzed by CeO<sub>2</sub> nanoparticles with different structures. Nanoflowers: 39.8% Ce(III) and 0.93 for M<sub>5</sub>/M<sub>4</sub>, nanoparticles: 39.9% Ce(III) and 0.93 for M<sub>5</sub>/M<sub>4</sub>.



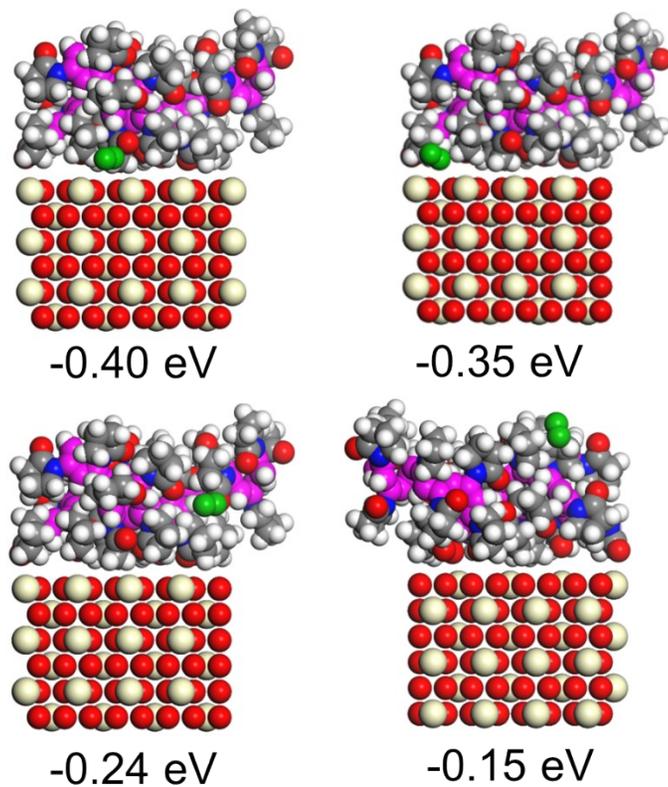
**Fig. S13** XPS spectra for (a) Ce 3d and (b) O 1s of the PVP-free CeO<sub>2</sub> nanocubes.



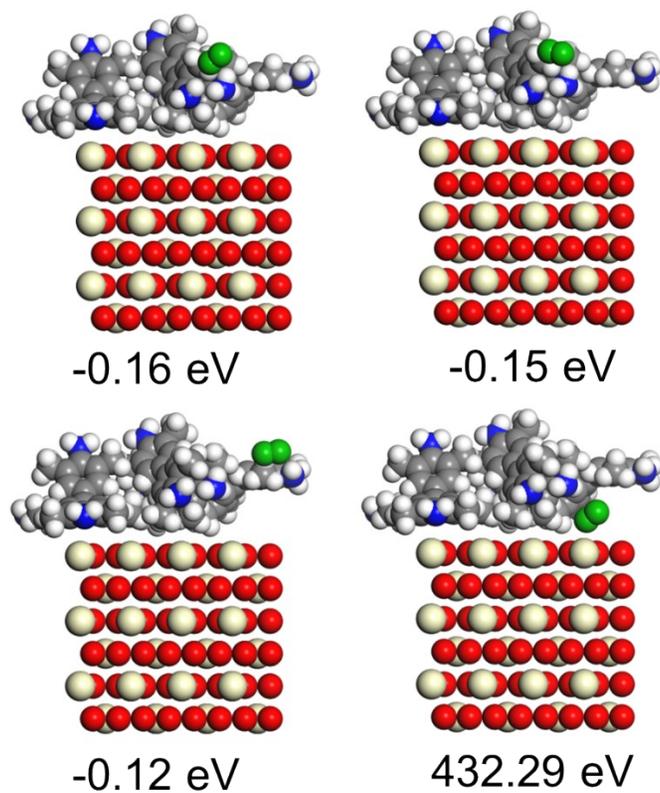
**Fig. 14** The adsorption energy of O<sub>2</sub> on the {220} facet in different configuration models. Green: O atoms within O<sub>2</sub>, red and light yellow: lattice O and Ce atoms within CeO<sub>2</sub>.



**Fig. 15** The adsorption energy of  $\text{O}_2$  (green) on the oxygen-deficient  $\{220\}$  facet in different configuration models. Green: O atoms within  $\text{O}_2$ , red and light yellow: lattice O and Ce atoms within  $\text{CeO}_2$ .



**Fig. 16** The adsorption energy of O<sub>2</sub> (green) on the oxygen-deficient {220} facet with the existence of PVP in different configuration models. Green: O atoms within O<sub>2</sub>; red: O atoms within CeO<sub>2</sub> and PVP; light yellow: lattice Ce atoms with CeO<sub>2</sub>; grey, blue and white: C, N and H atoms within PVP



**Fig. 17** The adsorption energy of O<sub>2</sub> (green) on the oxygen-deficient {220} facet with the existence of TMB in different configuration models. Green: O atoms within O<sub>2</sub>; red and light yellow: lattice O and Ce atoms within CeO<sub>2</sub>; grey, blue and white: C, N and H atoms within TMB.