Adsorption of C₂ Gases over CeO₂-based Catalysts: Synergism of Cationic Sites and Anionic Vacancies

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Supporting Information

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Figure S1: Spatial charge density distribution plots for the O-planes and Ce-planes constituting O and Ce ions of the surface layer of three CeO$_2$-based systems. (a) O-plane and Ce-plane of CeO$_2$, (b) O-plane and Ce-plane of CeO$_{2-\delta}$ and (c) O-plane and Ce-plane of Ce$_{1-x}$Pd$_x$O$_{2-\delta}$. Colour codes for the magnitude of charge density at a particular region are given at the bottom of the figure.
Figure S2: Spatial charge density distribution plots of the O-planes and Ce-planes of three CeO$_2$-based systems after C$_2$H$_2$ adsorption. (a) O-plane and Ce-plane CeO$_2$, (b) O-plane and Ce-plane of CeO$_{2-\delta}$ and (c) O-plane and Ce-plane of Ce$_{1-x}$Pd$_x$O$_{2-\delta}$. Colour key is same as that of Figure S1.
Figure S3: Spatial charge density distribution plots of the O-planes and Ce-planes of three CeO$_2$-based systems after C$_2$H$_4$ adsorption. (a) O-plane and Ce-plane of CeO$_2$, (b) O-plane and Ce-plane of CeO$_{2-\delta}$ and (c) O-plane and Ce-plane of Ce$_{1-x}$Pd$_x$O$_{2-\delta}$. Colour key is same as that of Figure S1.
Figure S4: Spatial charge density distribution plots of the O-planes and Ce-planes of three CeO$_2$-based systems after C$_2$H$_6$ adsorption. (a) O-plane and Ce-plane of CeO$_2$, (b) O-plane and Ce-plane of CeO$_{2-\delta}$ and (c) O-plane and Ce-plane of Ce$_{1-x}$Pd$_x$O$_{2-\delta}$. Colour key is same as that of Figure S1.