Electronic Supplementary Material (ESI) for Faraday Discussions.

The electronic properties of Au clusters on CeO_2(110) surface with and without O-defects

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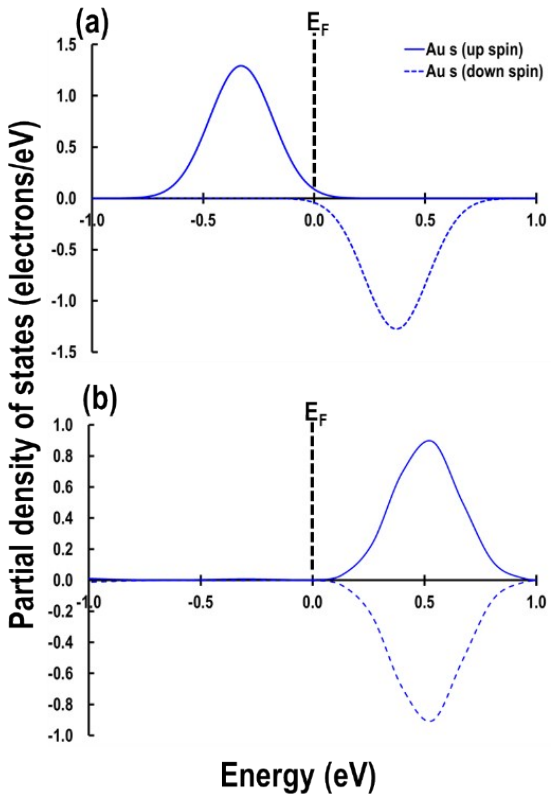

Figure S1. Partial density of states of (a) Au atom and (b) Au atom in O…O_{bridge} model.

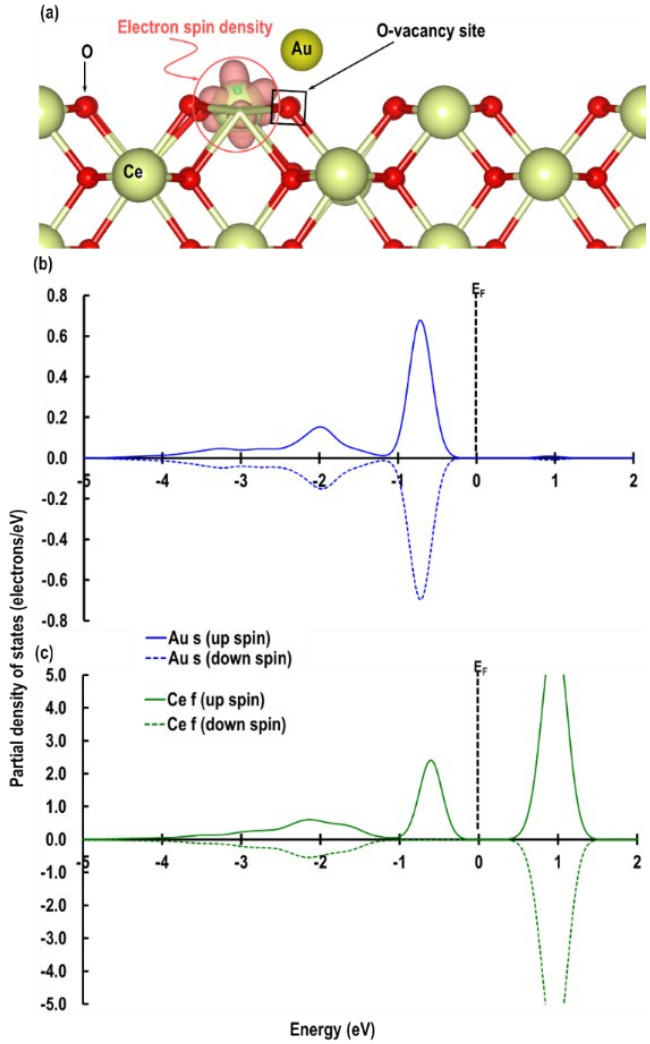

Figure *S2*. (a) Electron spin density for the system of a Au atom adsorbed on top of an O-vacancy (shown as a black transparent box) with five atomic layered CeO_2(110) (3×3) surface model. In this calculation we adsorb the Au atom only on one side of the two exposed surfaces, partial

density of states (b) for the Au atom adsorbed on top of an O-vacancy and (c) for the reduced Ce on the CeO_2(110) surface close to the O-vacancy.

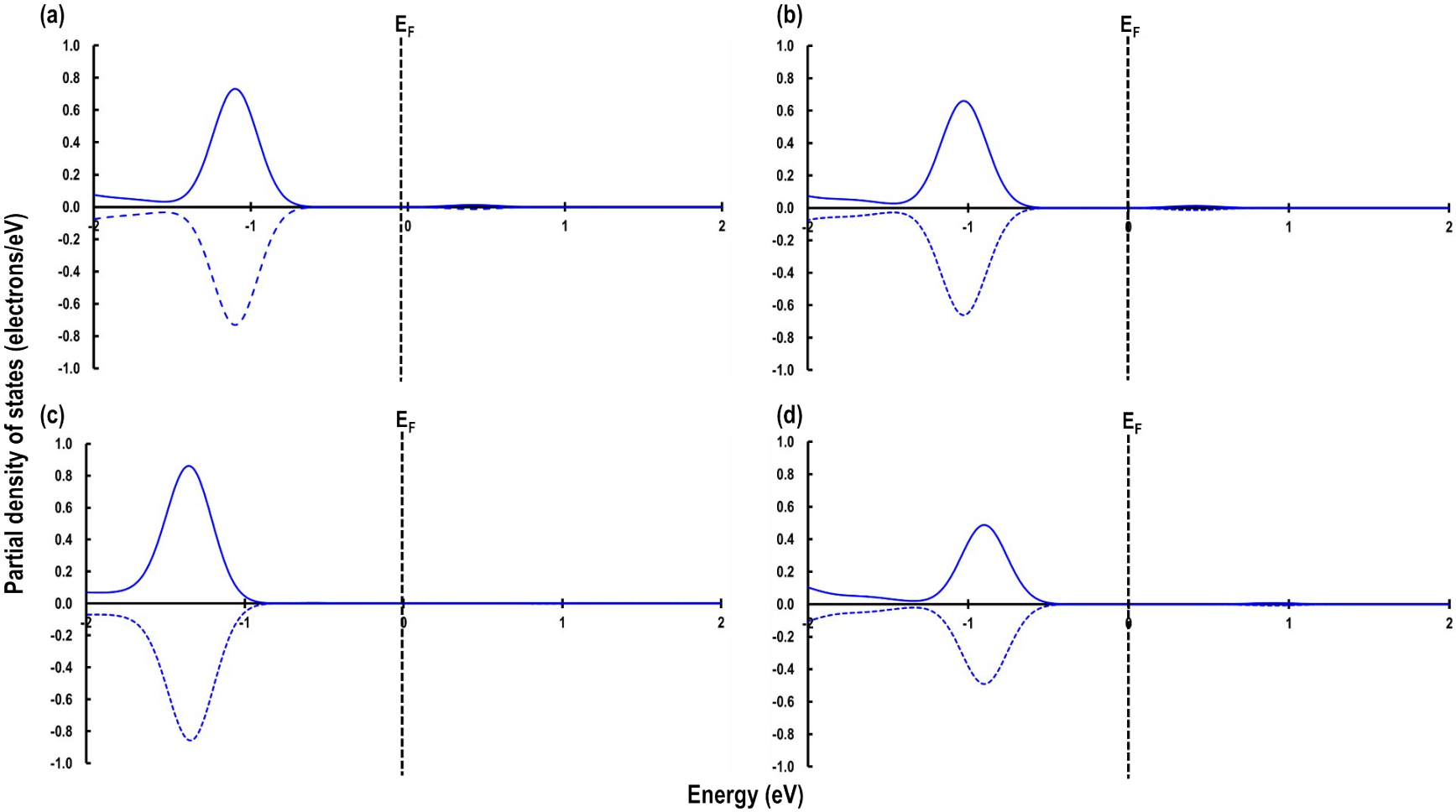

Figure S3. (a) Au *s*-orbital signatures for model with two water molecules obtained by DFT+U calculations. Au *s*-orbital signatures for the models with (b) two, (c) four and (d) six water molecules obtained by DFT+U+D3 calculations.