

# Supporting Information

## Tuning the Surface Properties of AuPd Nanoparticles for Adsorption of O and CO

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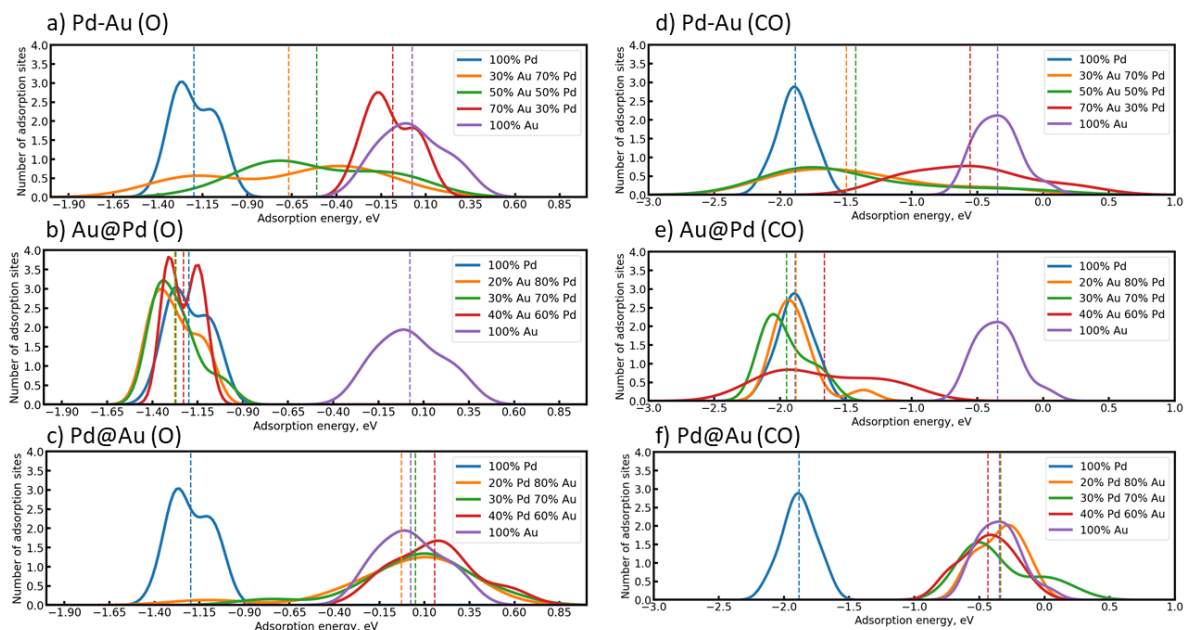


Figure S1: Distributions of adsorption energies of O and CO species calculated for 14 symmetrical nonequivalent adsorption sites on fcc alloy and core-shell Pd@Au and Au@Pd nanoparticles and alloy Pd-Au nanoparticles. The distributions were obtained by applying 0.35 eV smearing to the calculated adsorption energies. The dashed lines reflect the average adsorption energies calculated for each distribution.

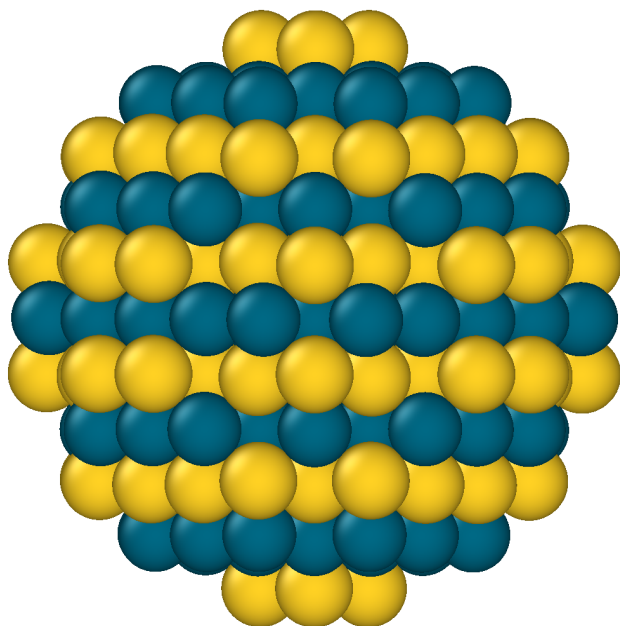


Figure S2: PdAu nanoparticle with L1<sub>1</sub> structure

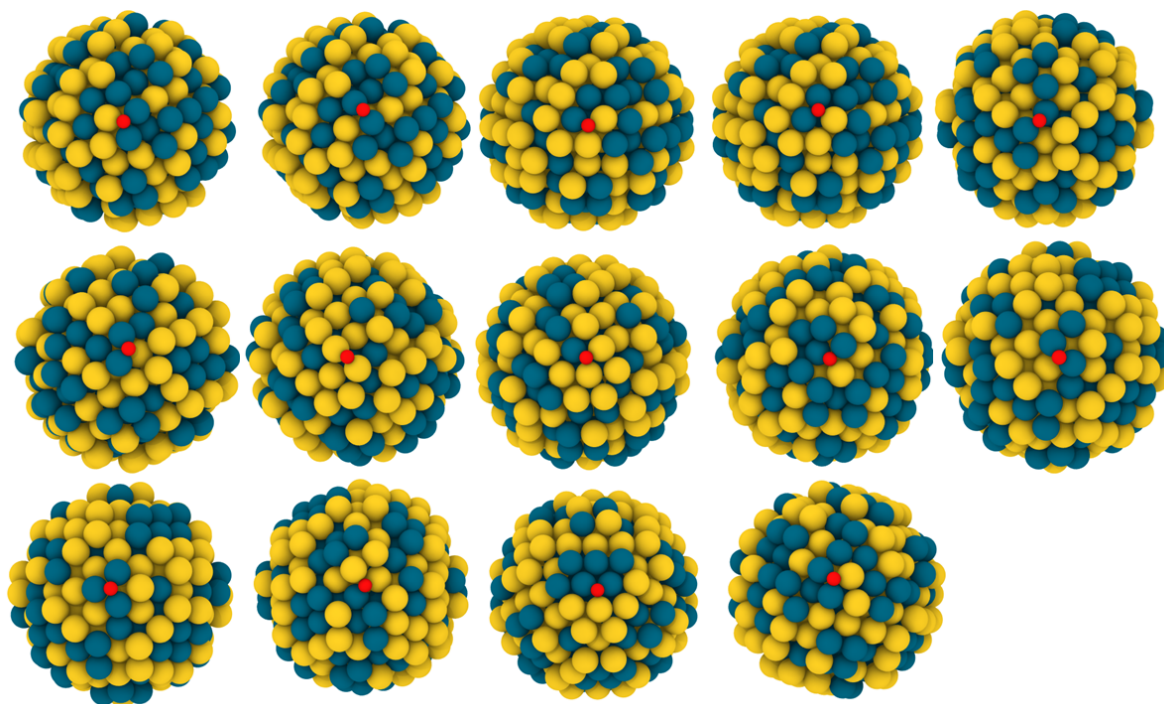


Figure S3: Adsorption sites for O

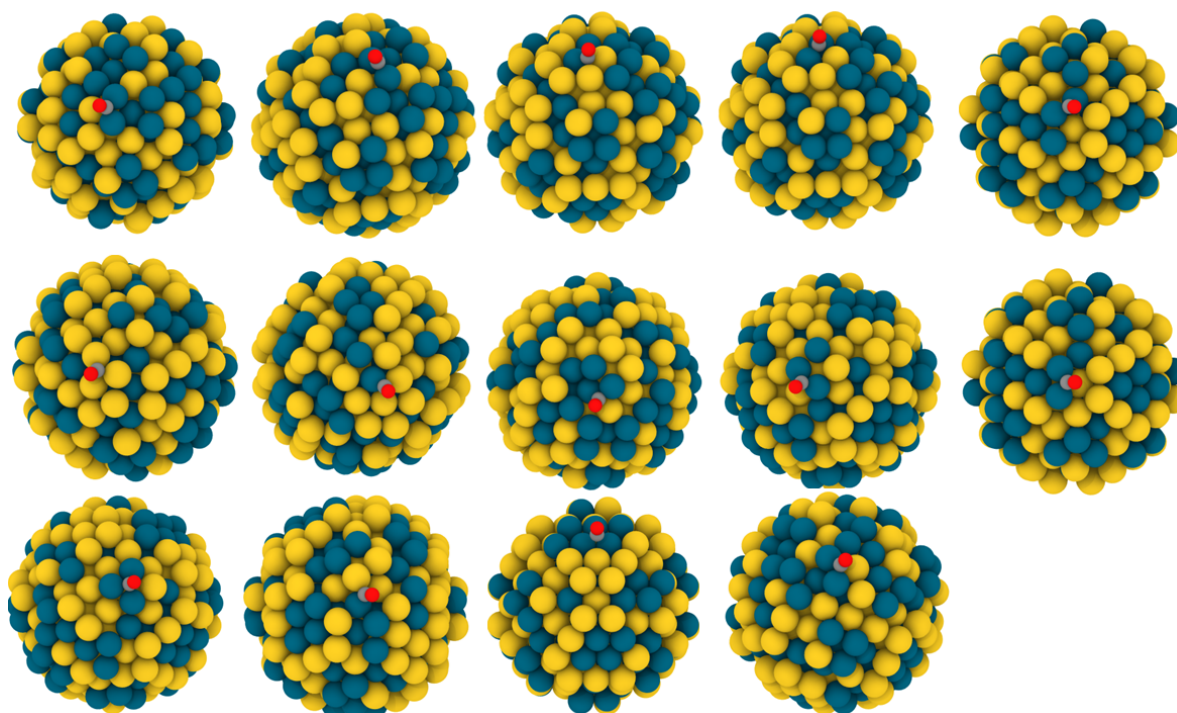


Figure S4: Adsorption sites for CO