

Electronic Supporting Information for:

Insights into the growth of nanoparticles in liquid polyol by thermal annealing

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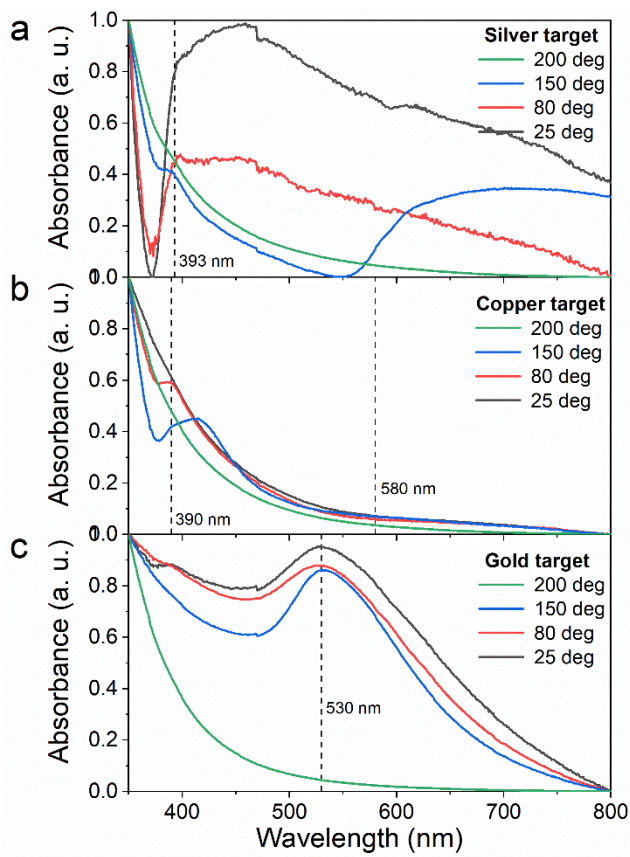


Figure S1. Absorption spectra in absolute intensity scale of diluted PEEL solution after sputtering of the (a) silver target, (b) copper target, (c) and gold target in their pristine state (black curve) and after annealing at 80 °C (red), 150 °C (blue) and 200 °C (green) during 5h.

Supplementary information 1: Details of the DFT calculation

Generation of model surfaces

The pure and oxidized metal surfaces representing different facets of nanoparticles were generated from the bulk using orthogonal unit cells, with enough surface area to prevent intermolecular interactions between PEEL molecules on the surface. The face centered cubic structure with lattice parameters used to model a N-layer slab exposing the desired facet surface and its lattice parameters a and b are summarized in Table S1.

Nature of the surface	a (bulk), Å	Facet	Number of layers	a , Å	b , Å
Au	4.23	111	5	11.96	10.37
		110	5	12.69	11.96
		100	6	12.69	12.69
Ag	4.09	111	5	11.55	10.00
		110	5	12.56	11.84
		100	6	12.56	12.56
Cu	3.73	111	5	10.54	13.70
		110	5	11.18	10.54
		100	6	11.18	11.18
Cu ₂ O	4.45	111	5	12.58	10.89
		110	4	13.34	12.58
		100	5	13.34	13.34

Table S1.

Relaxed interface geometry

Relaxed interface geometries for the pentaerythritol molecule (PE, a simplified version of PEEL) on the various surfaces considered in the manuscript can be found below.

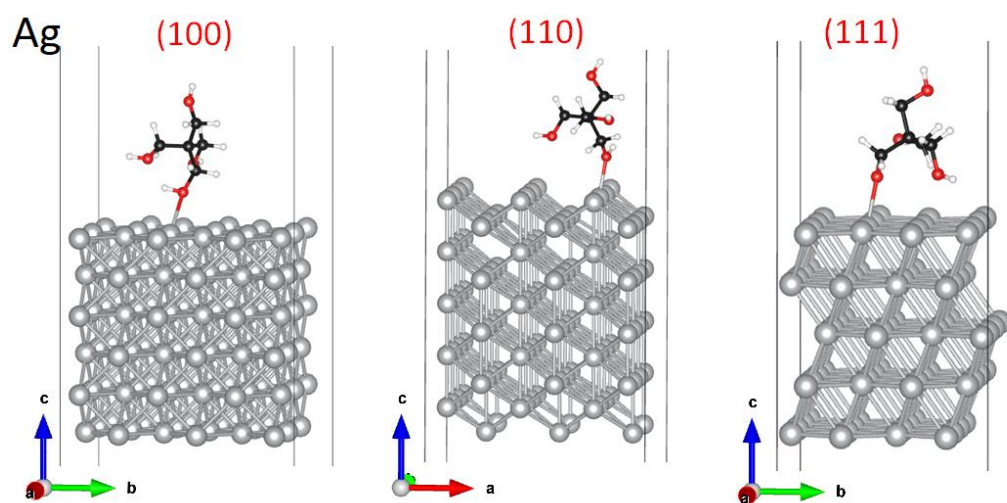


Figure S2. Side view of the final relaxed structure for PE adsorbed on Ag (100), (110) and (111) facets.

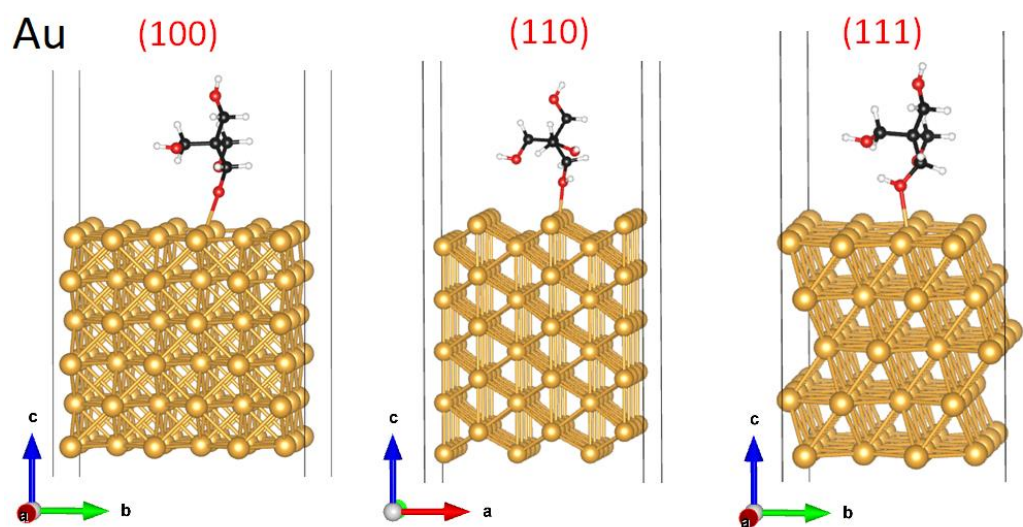


Figure S3. Side view of the final relaxed structure for PE adsorbed on Au (100), (110) and (111) facets.

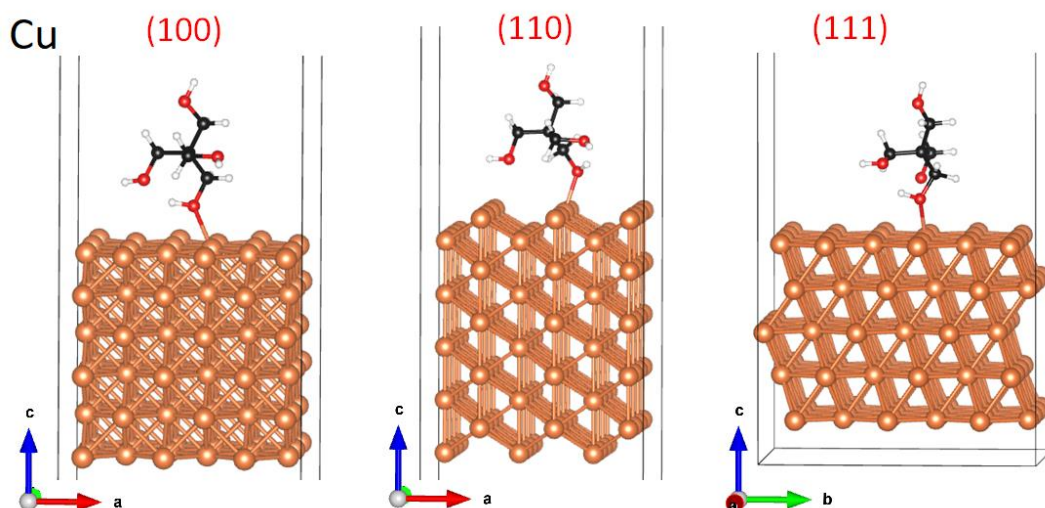


Figure S4. Side view of the final relaxed structure for PE adsorbed on Cu (100), (110) and (111) facets.

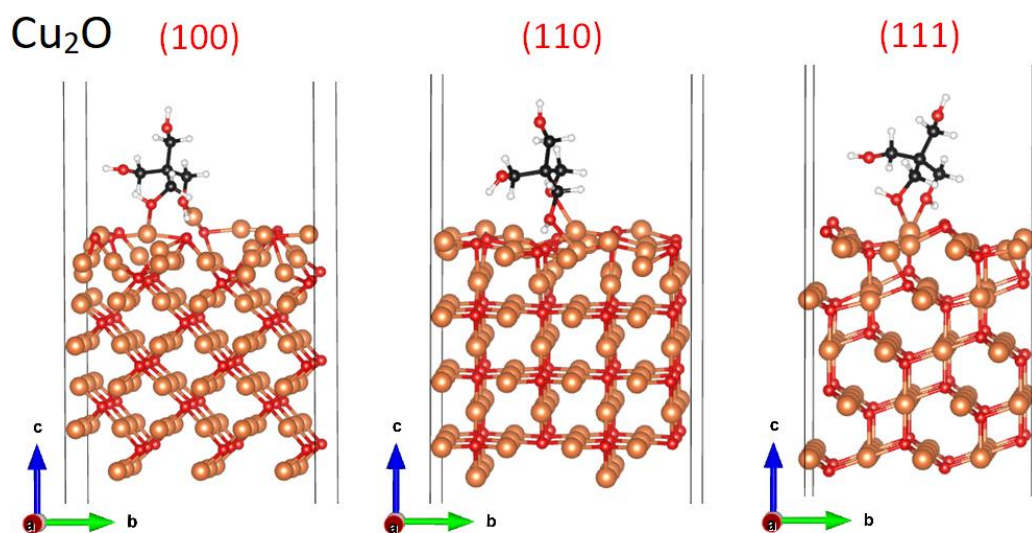


Figure S5. Side view of the final relaxed structure for PE adsorbed on Cu₂O (100), (110) and (111) facets.