

## **Supporting Information**

for

## Atomistic insights into the morphological dynamics of gold and platinum nanoparticles: MD simulations in vacuum and aqueous media

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**Additional figures** 

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**Figure S1:** Visualization of Au NPs with diameters of 2 nm (panels A and B) and 8 nm (panels C and D) at 100 K (panels A and C) and 1100 K (panels B and D).



**Figure S2:** Visualization of Pt NPs with diameters of 2 nm (panels A and B) and 8 nm (panels C and D) at 100 K (panels A and C) and 2000 K (panels B and D).



**Figure S3:** Temperature dependence of surface area to volume ratio for Au (panel a) and Pt (panel b) NPs. The NP diameters range from 1 nm to 8 nm. The symbols for the NP diameters are explained in Figure S4.



**Figure S4:** Temperature dependence of the average surface potential energy per atom for Au (panel a) and Pt (panel b) NPs. The NP diameters range from 1 up to 8 nm.