Supporting Information

Theoretical design of platinum-sliver single atom alloy catalyst with CO adsorbate-induced surface structures

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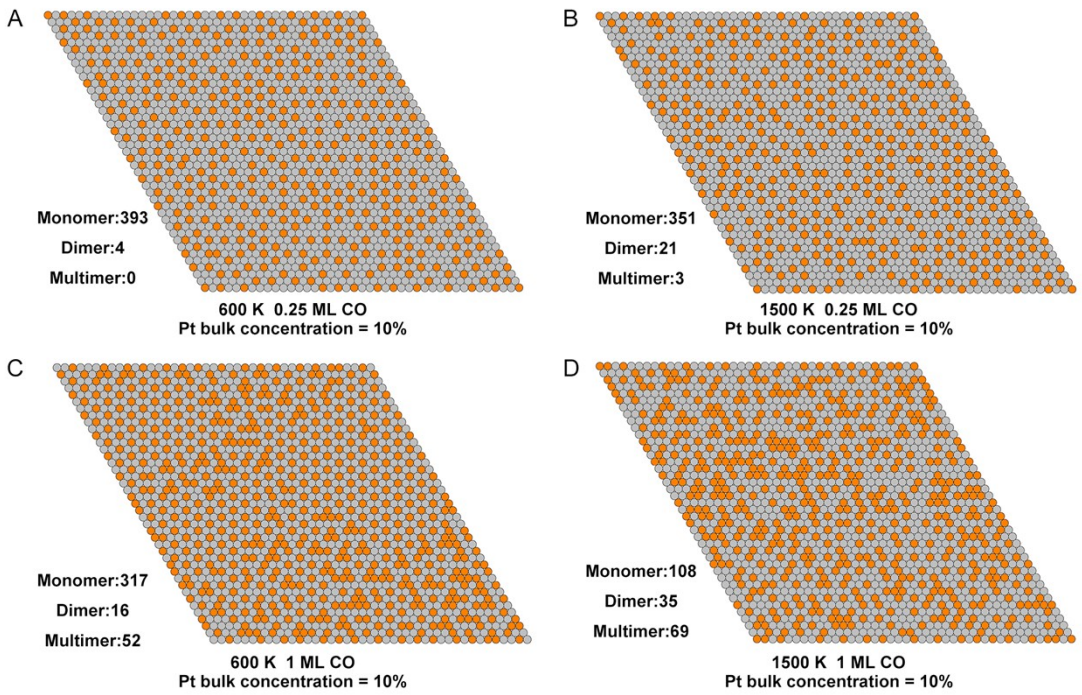

Figure S1 MC snapshots of the atomic structures of CO/Vac-Pt/Ag(111) with 10% Pt and CO coverage of 0.25ML and 1 ML at 600 K and 1500 K.

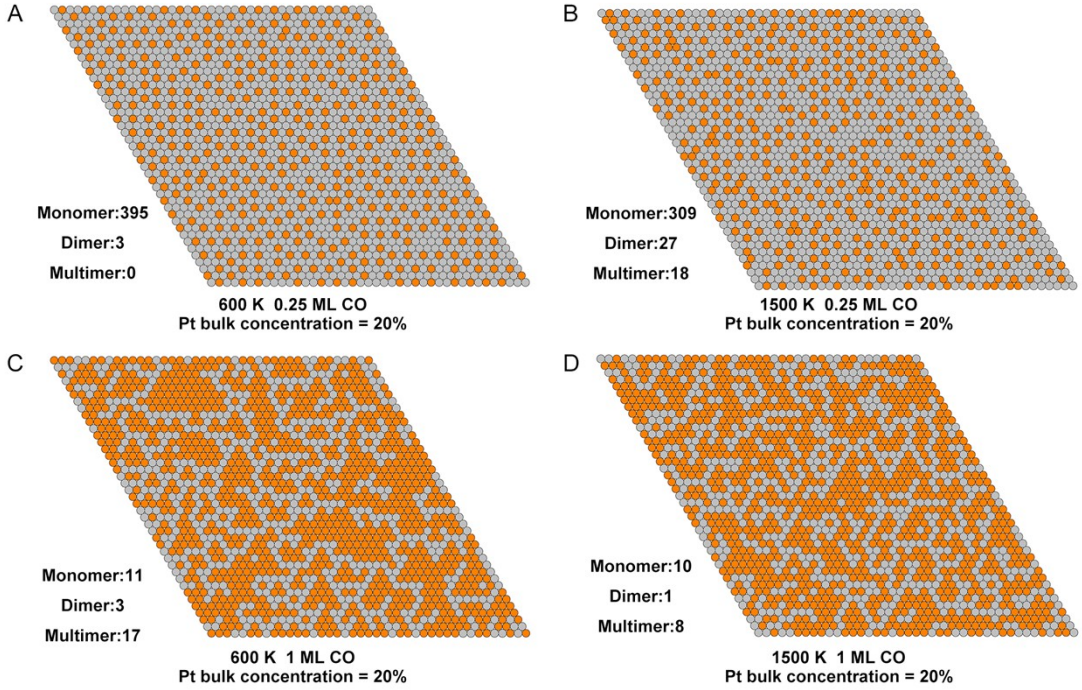

Figure S2 MC snapshots of the atomic structures of CO/Vac-Pt/Ag(111) with 20% Pt and CO coverage of 0.25ML and 1 ML at 600 K and 1500 K.

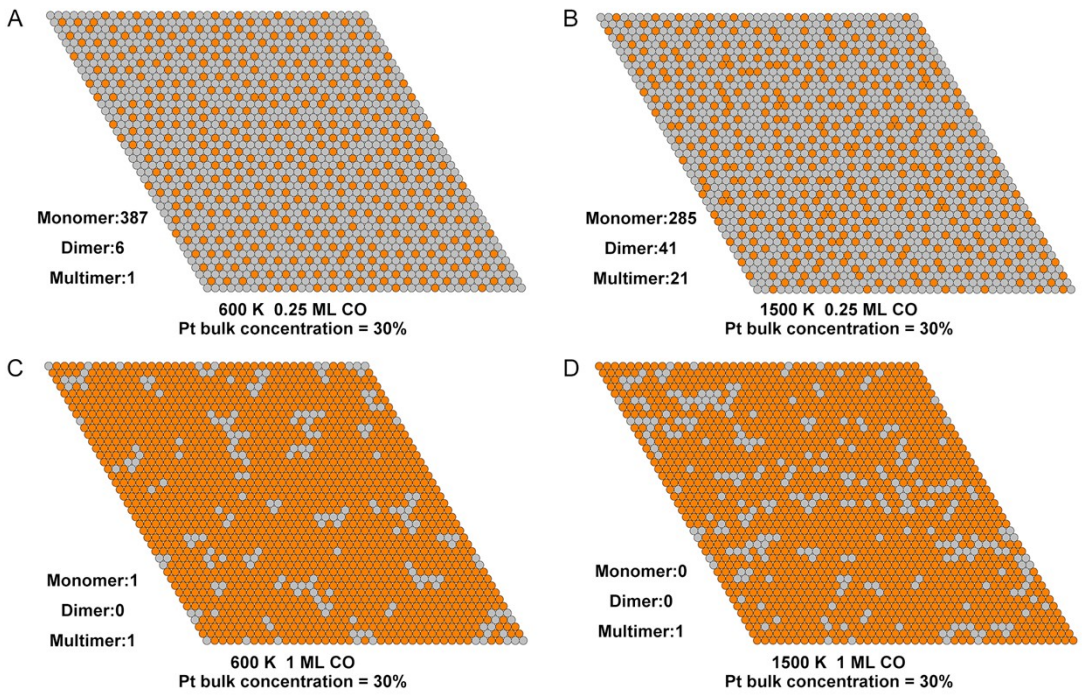

Figure S3 MC snapshots of the atomic structures of CO/Vac-Pt/Ag(111) with 30% Pt and CO coverage of 0.25ML and 1 ML at 600 K and 1500 K.

Table S1 The free energies of the four e- ORR reactions on Pd3Ag(111) surface without and with solvent, as well as the corresponding theoretical limiting potential and overpotential.

Surface model	$\Delta G_1(eV)$	$\Delta G_2(eV)$	$\Delta G_3(eV)$	$\Delta G_4(eV)$	$U_L(V)$	$\eta(V)$
without solvent	−1.01	−2.19	−0.91	−0.82	0.82	0.41
with solvent	−1.24	−1.95	−0.94	−0.79	0.79	0.44