Supporting Information
for the article

Shielding the chemical reactivity using graphene layers for controlling the surface properties of carbon materials

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CONTENT

Table S1. Binding energies (ΔE, kcal/mol), atomic charges and interatomic distances for coronene and circum-coronene complexes.

Number of carbon layers, n		**0**	**1**	**2**	**3**
ΔE, kcal/mol[1]	C_{24}	-120.7	-98.1	-67.9	-82.5
$C_{(C=O)}$ charge[2]	C_{54}	+0.236	+0.305	+0.311	+0.317
	C_{24}	+0.106 *-0.039*	+0.220 *-0.078*	+0.253 *-0.092*	+0.267 *-0.099*
O charge[2]	C_{54}	-0.127	-0.200	-0.224	-0.237
	C_{24}	-0.055 *+0.170*	-0.122 *+0.085*	-0.189 *+0.060*	-0.216 *+0.045*
Pd charge[2]	C_{54}	+1.333	+1.439	+1.401	+1.376
	C_{24}	+1.716 *+0.722*	+1.552 *+0.576*	+1.376 *+0.515*	+1.320 *+0.486*
Total PdCO charge[3]	C_{54}	+1.442	+1.544	+1.488	+1.456
	C_{24}	+1.767 *+0.853*	+1.650 *+0.583*	+1.440 *+0.483*	+1.587 *+0.432*

[1] The values for coronene based systems at PM6-D3H4 level; [2] The values of the Mulliken charges. The regular font is used for PM6-D3H4 level and the italic font is used for RI PBE level. For the coronene systems the total geometry optimization were carried out by RI PBE def2-SVP ZORA method and single point calculations by PM6-D3H4 method; for the circum-coronene systems the total geometry optimization at the PM6-D3H4 level were performed. [3] The sum of charges of the Pd, C and O atoms.

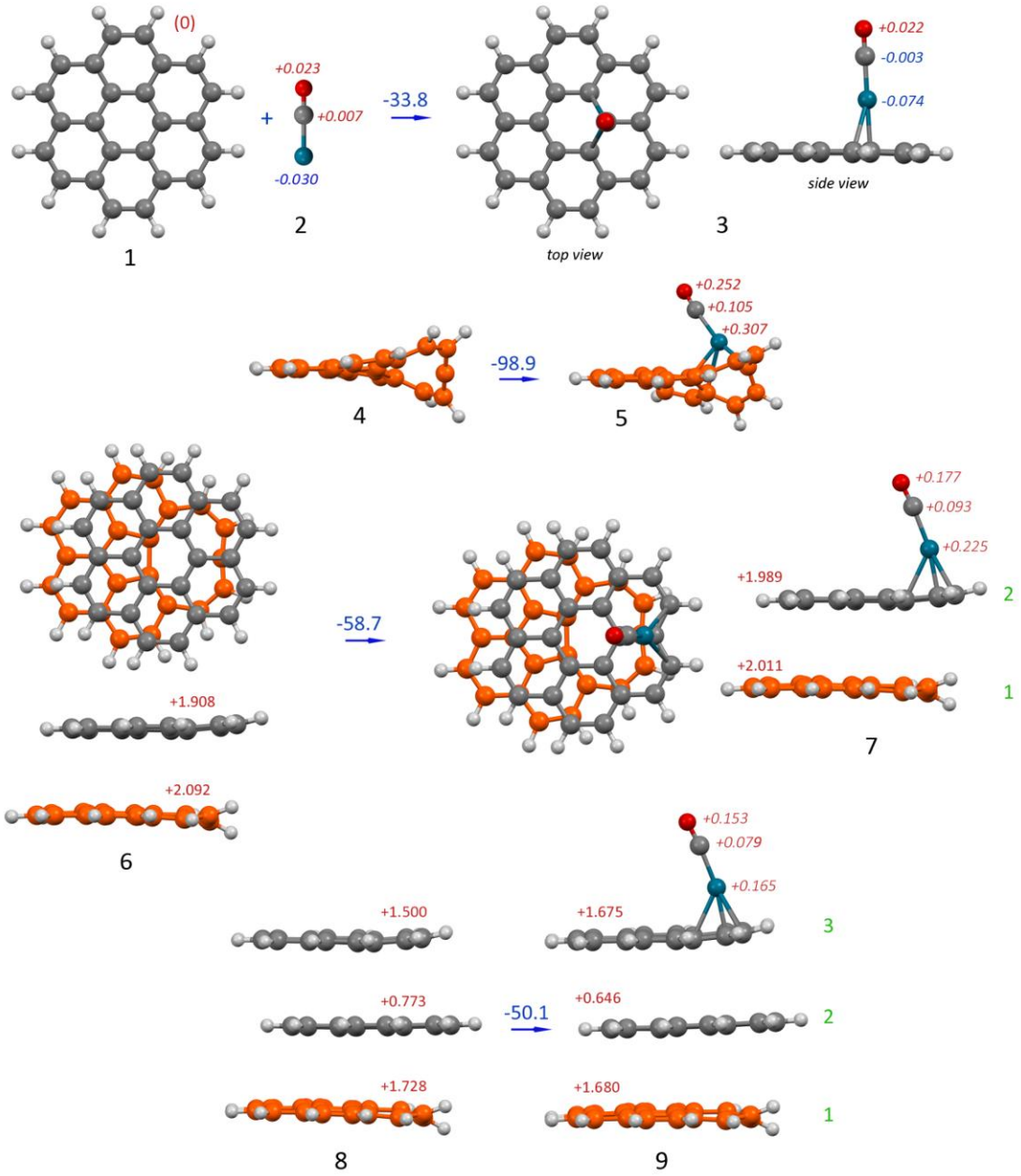

Figure S1. Neutral coronene molecule and complex (1, 3) and 4+ charged molecular structures (4-9) with single atomic defect optimized at RI PBE def2-SVP def2-SVP/J level. The Loewdin charges of each coronene sheet are denoted by red color and regular font; the atomic charges of the PdCO species are denoted by italic font; the reaction energies (kcal/mol) are denoted by blue color above the arrows and the numbers of sheets are denoted by green color. The sheet with defect is colored by orange color.

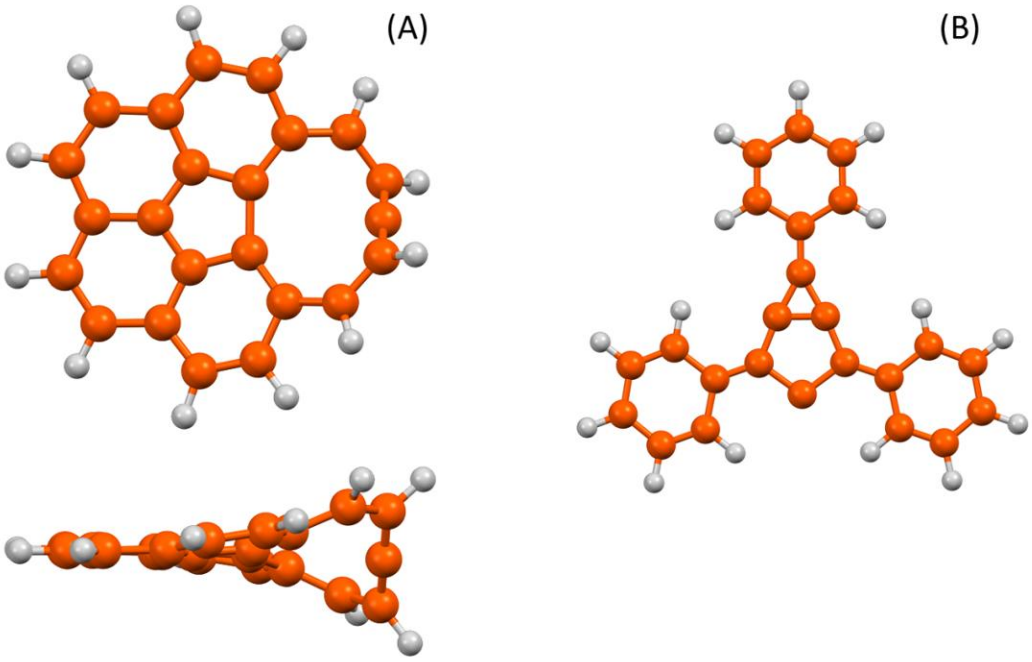

Figure S2. Optimized molecular structures of the coronene molecule with 4+ charged defect (RI PBE def2-SVP def2-SVP/J) and $Ph_3C_6^{(3+)}$ cation (PM6-D3H4).

Figure S3. Enlarged image of the figure 1A.

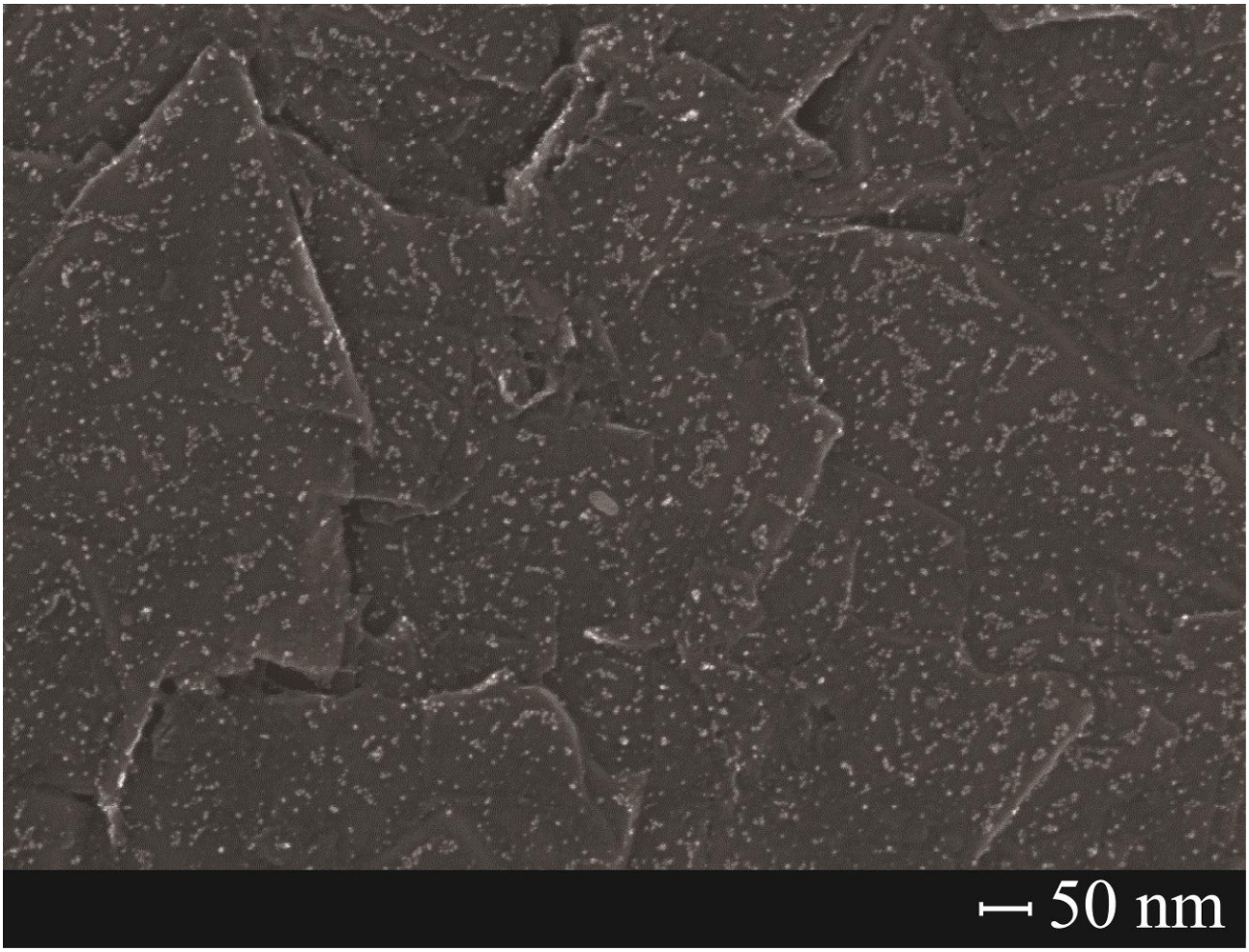

Figure S4. Enlarged image of the figure 1B.

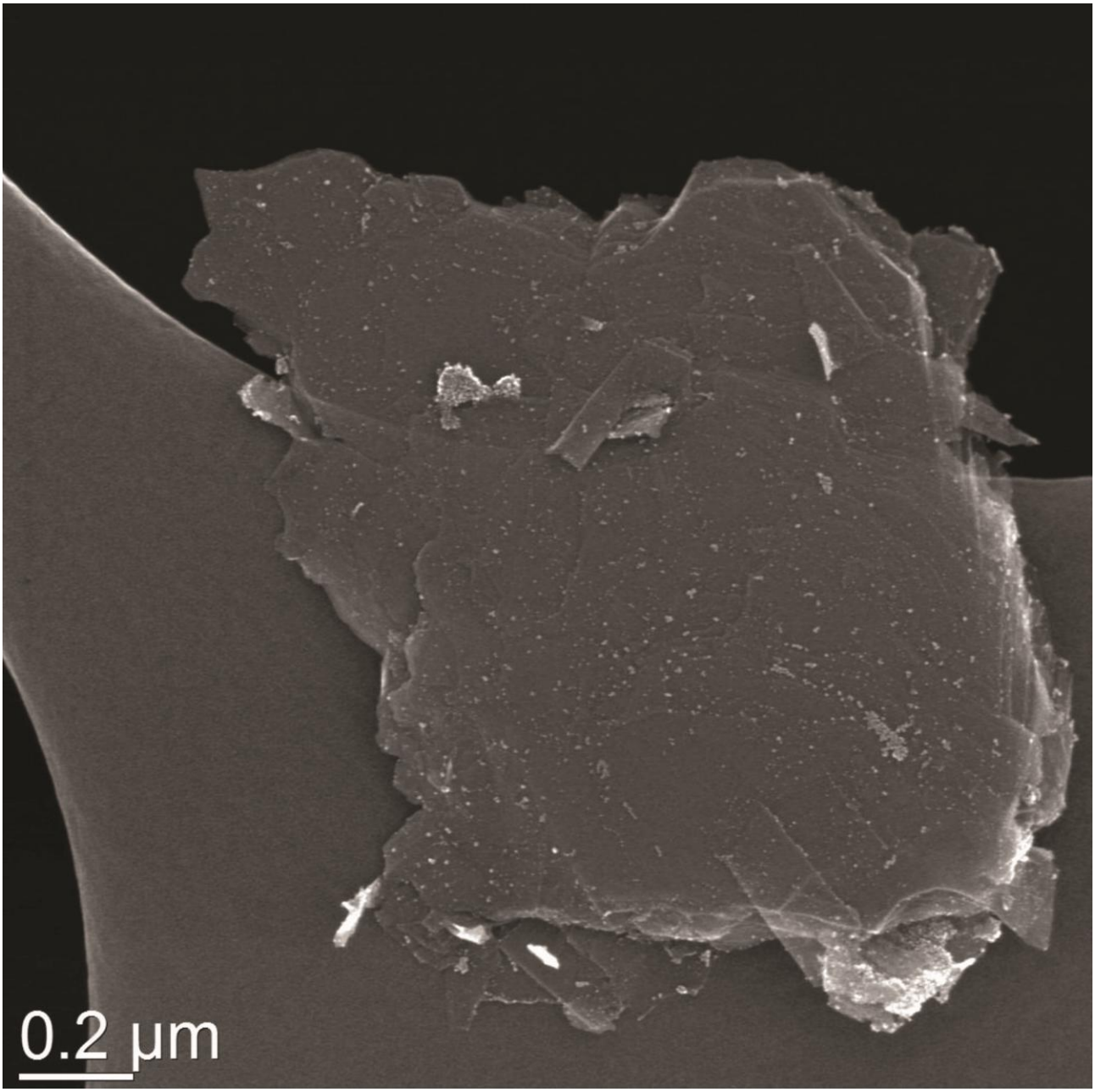

Figure S5. Enlarged image of the figure 2A.

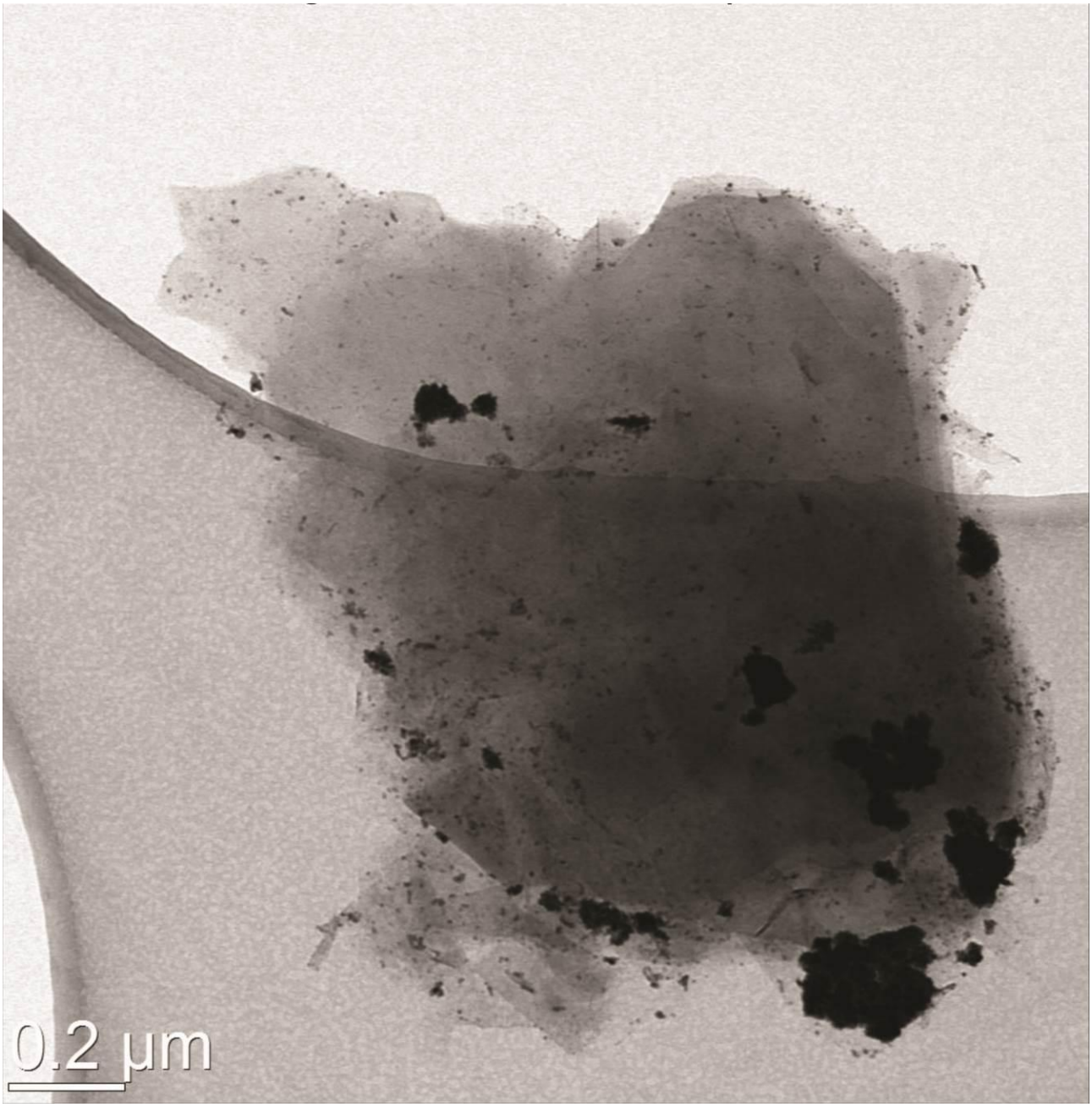

Figure S6. Enlarged image of the figure 2B.

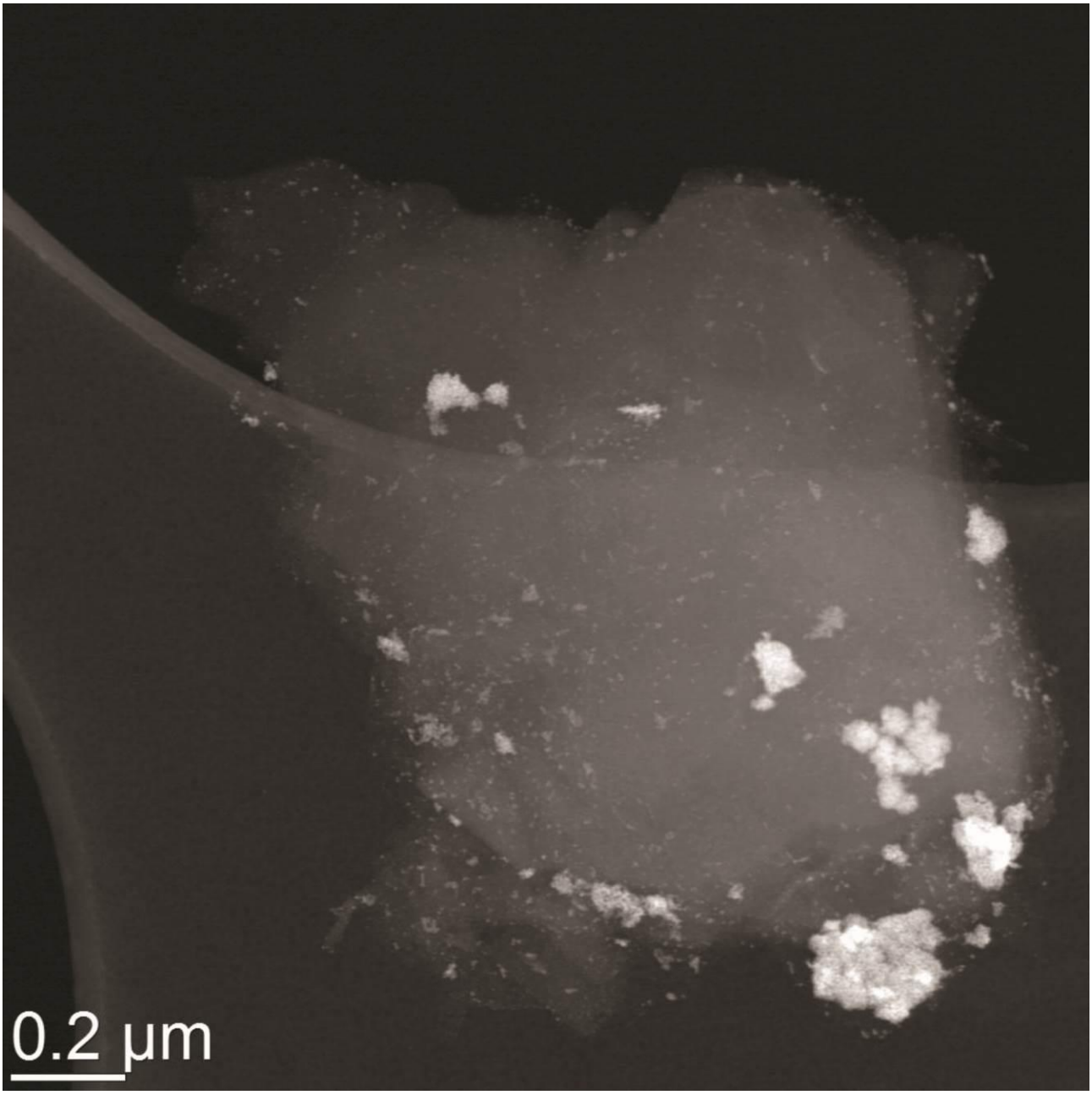

Figure S7. Enlarged image of the figure 2C.

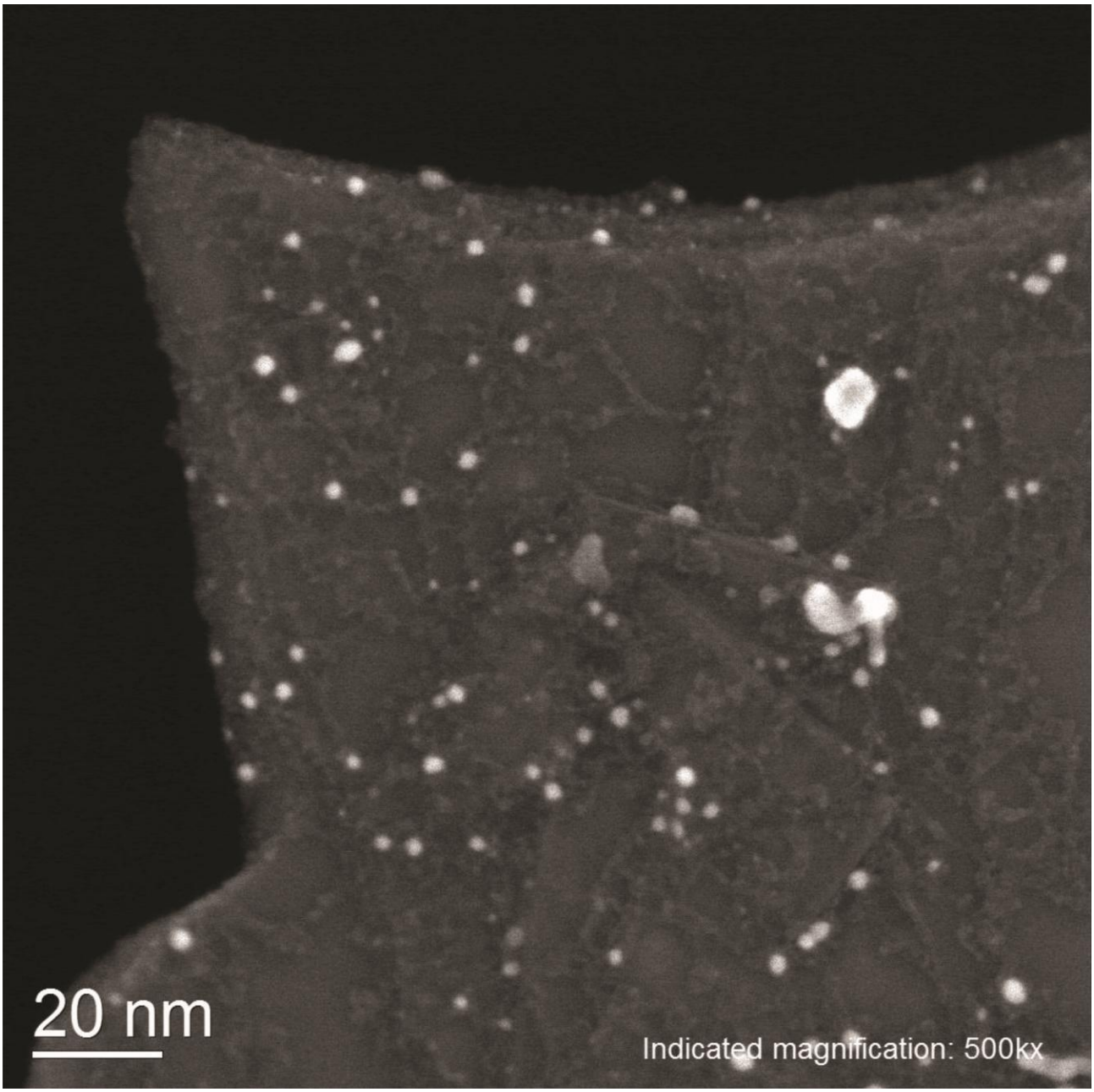

Figure S8. Enlarged image of the figure 2D.

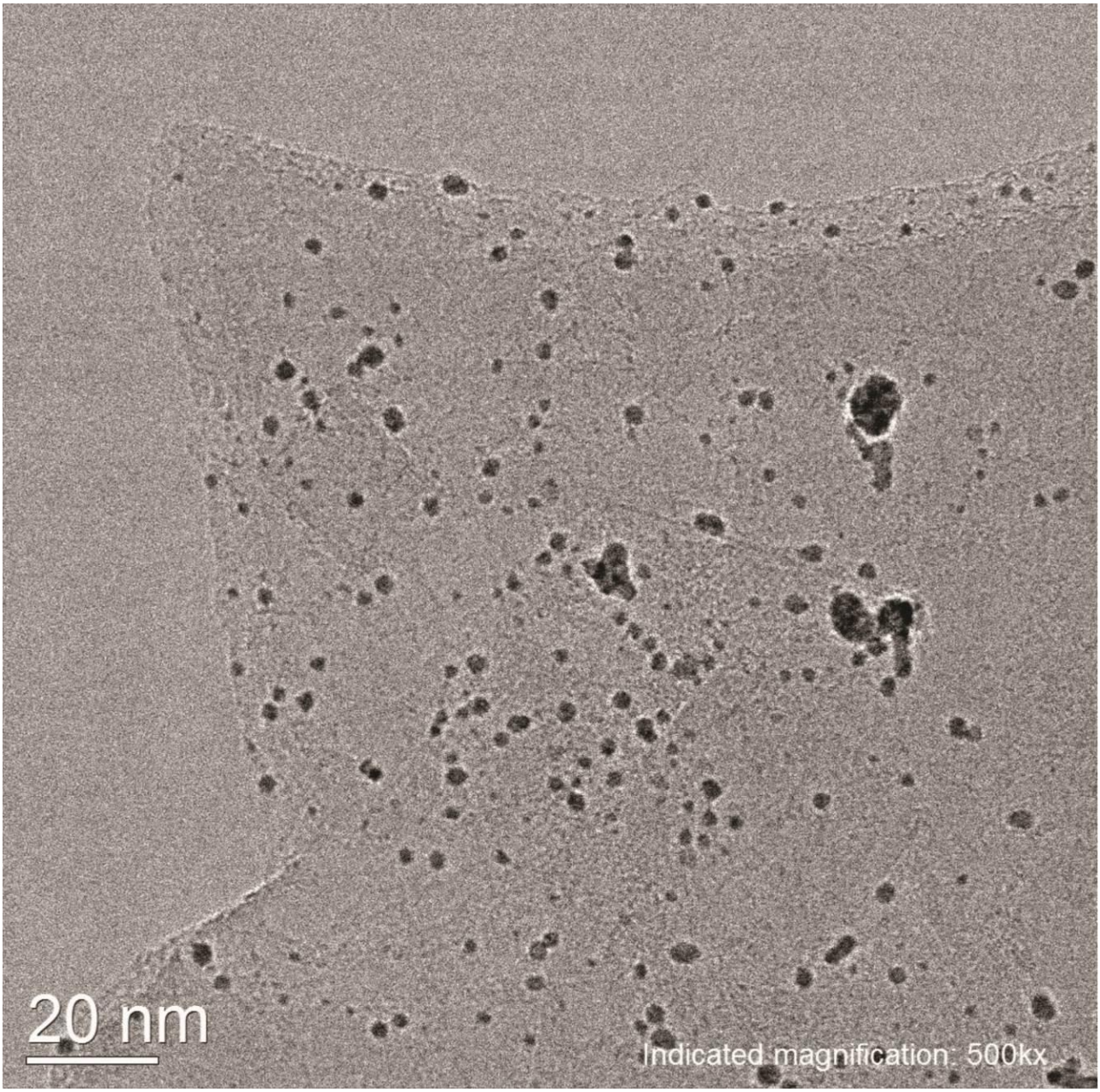

Figure S9. Enlarged image of the figure 2E.

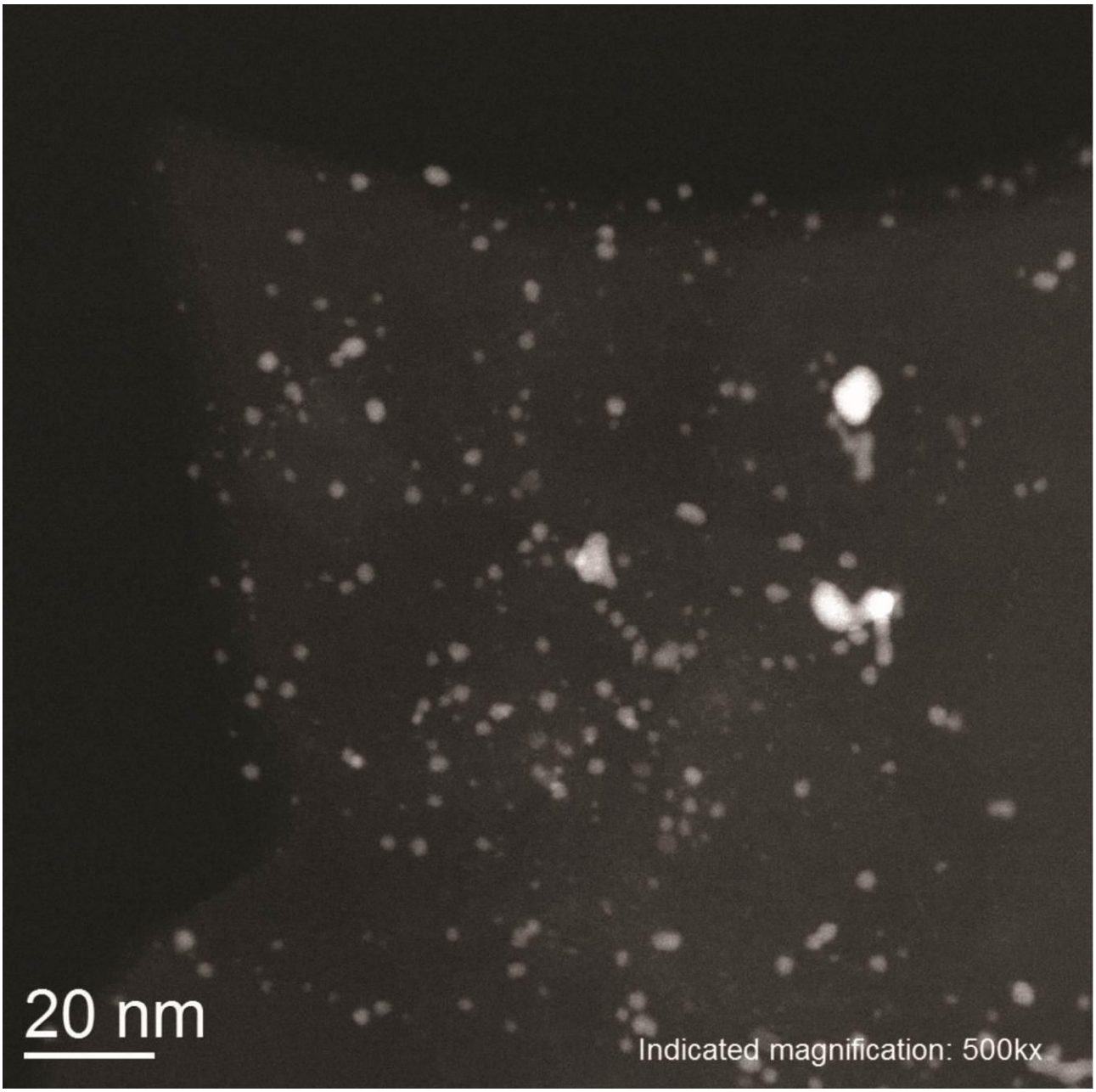

Figure S10. Enlarged image of the figure 2F.

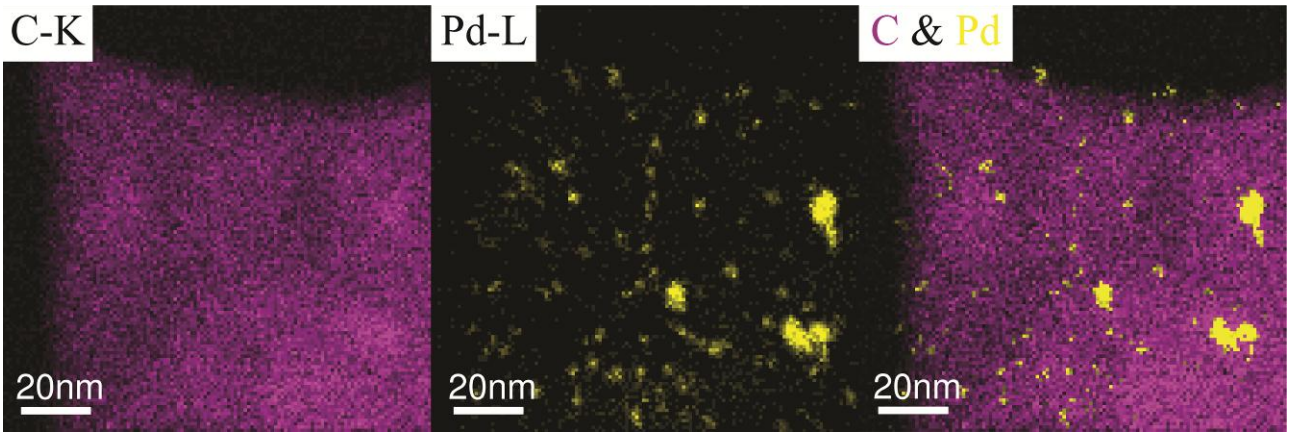

Figure S11. Enlarged image of the figure 2G.

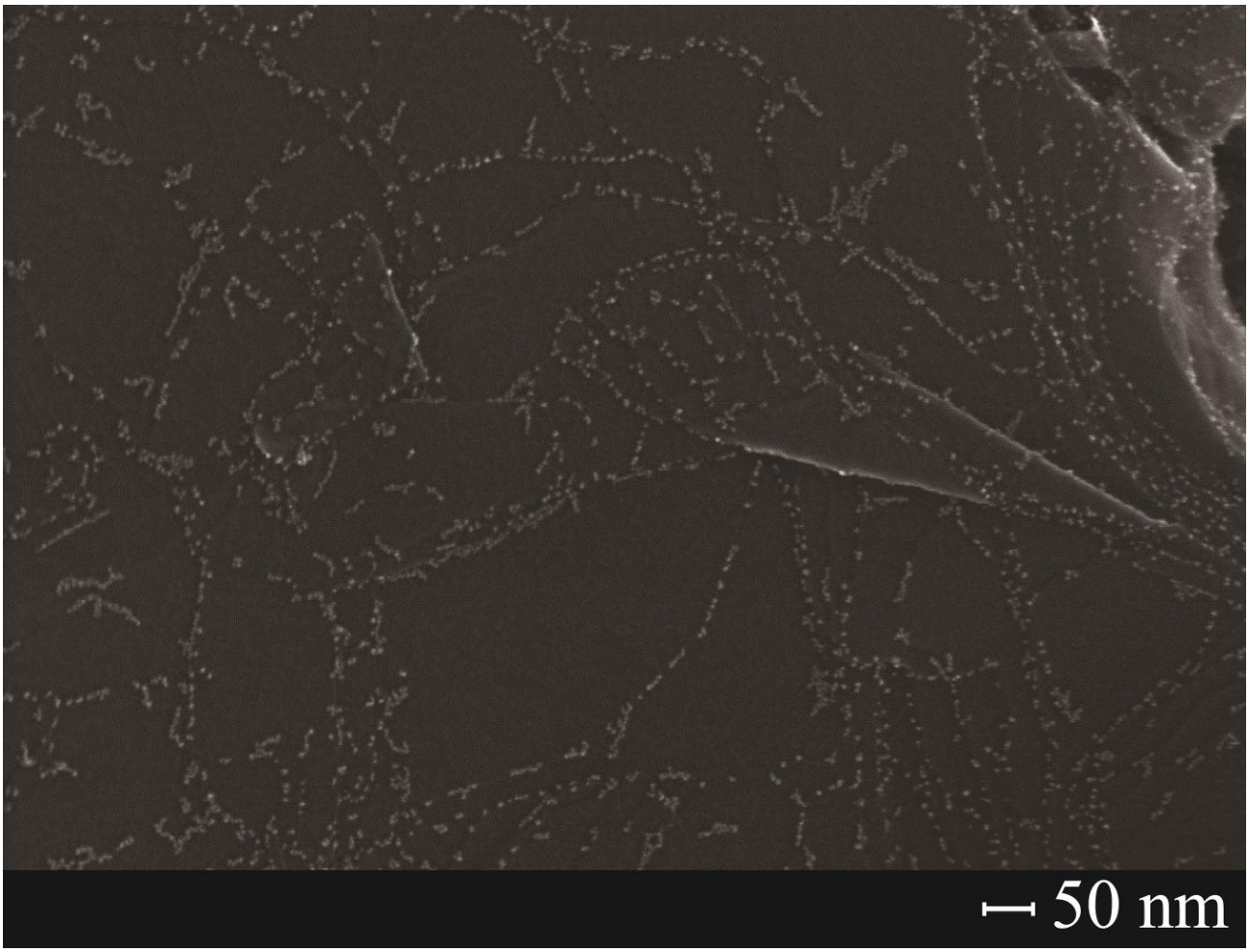

Figure S12. Enlarged image of the figure 6A.

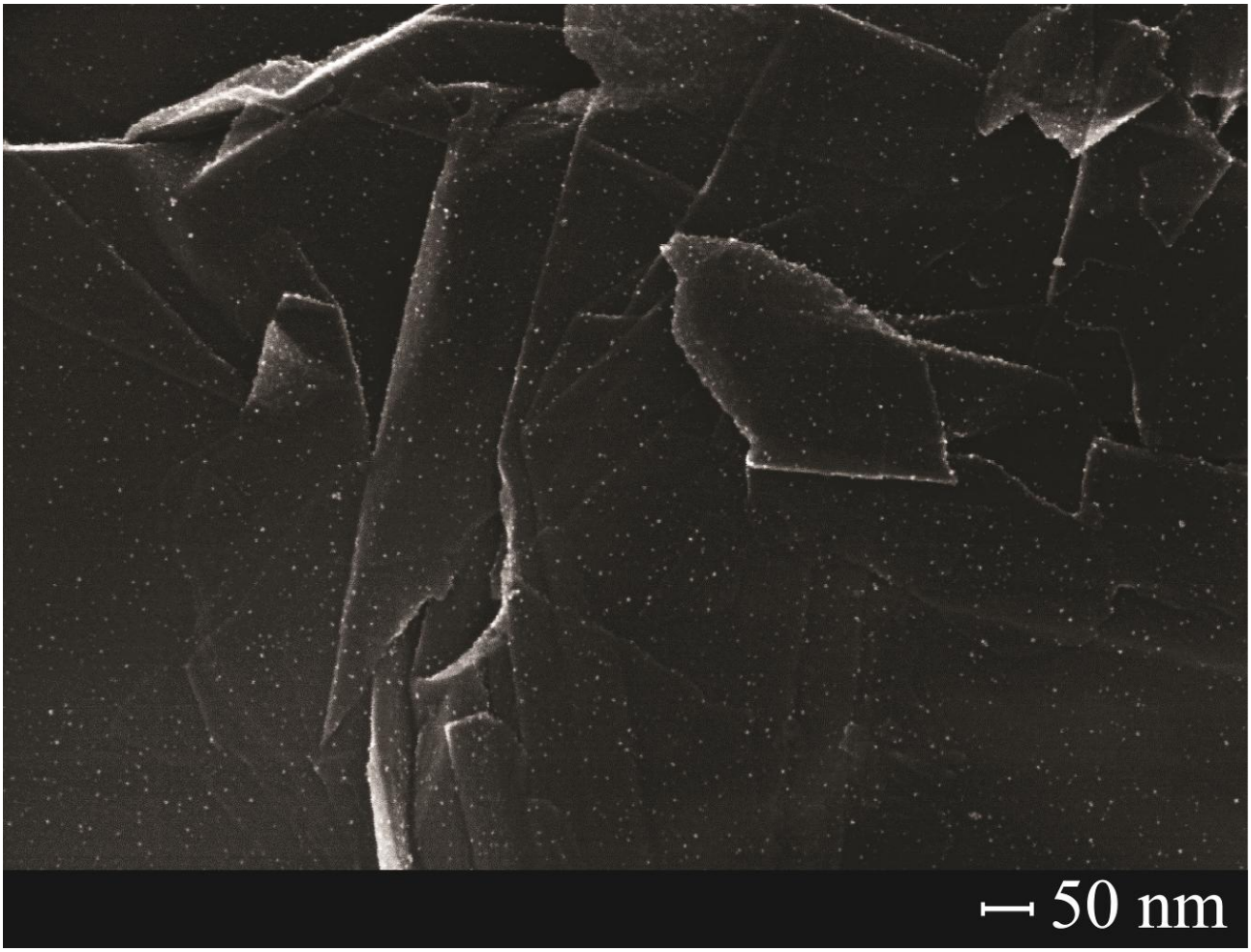

Figure S13. Enlarged image of the figure 6B.

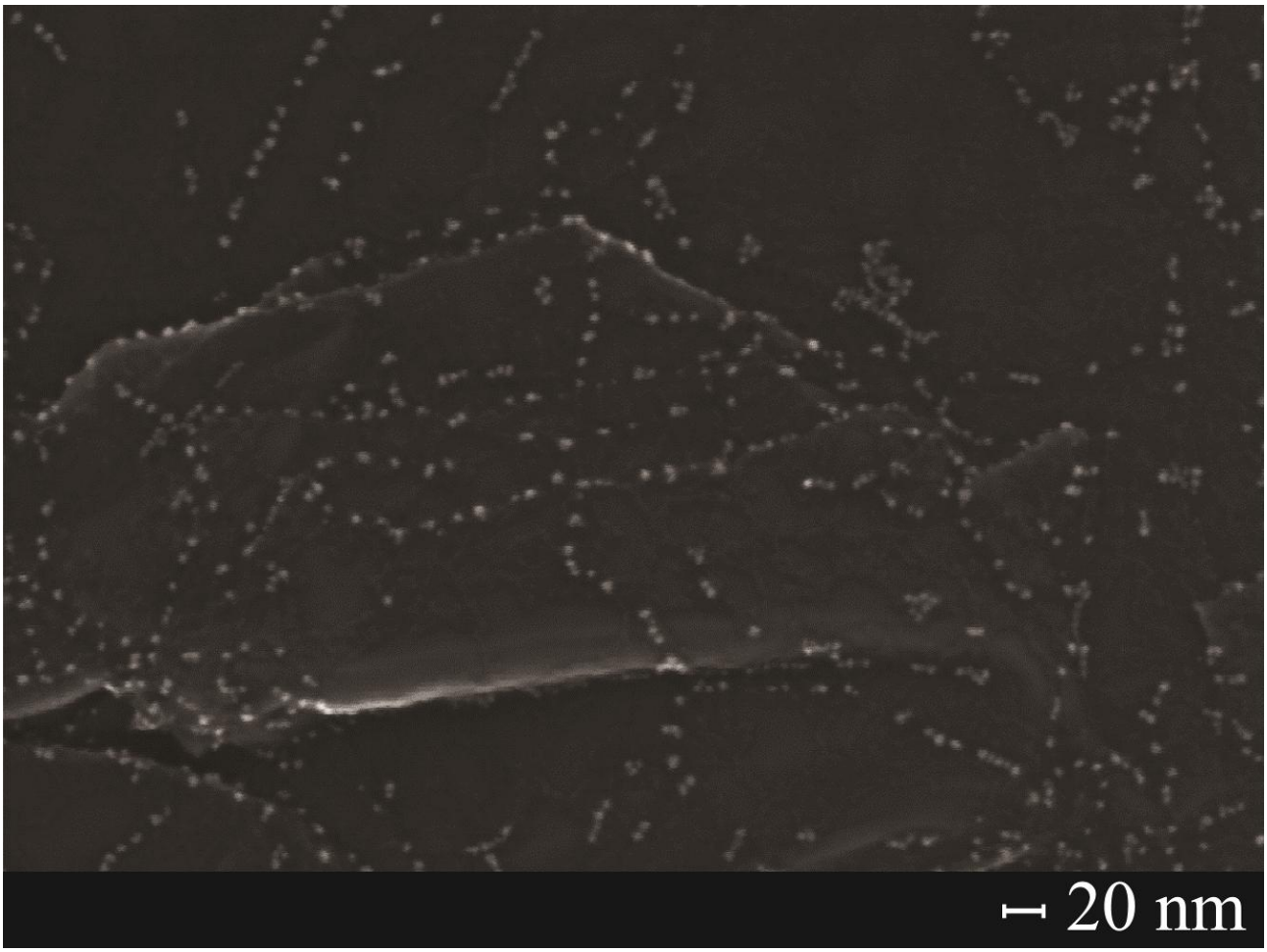

Figure S14. Enlarged image of the figure 6C.

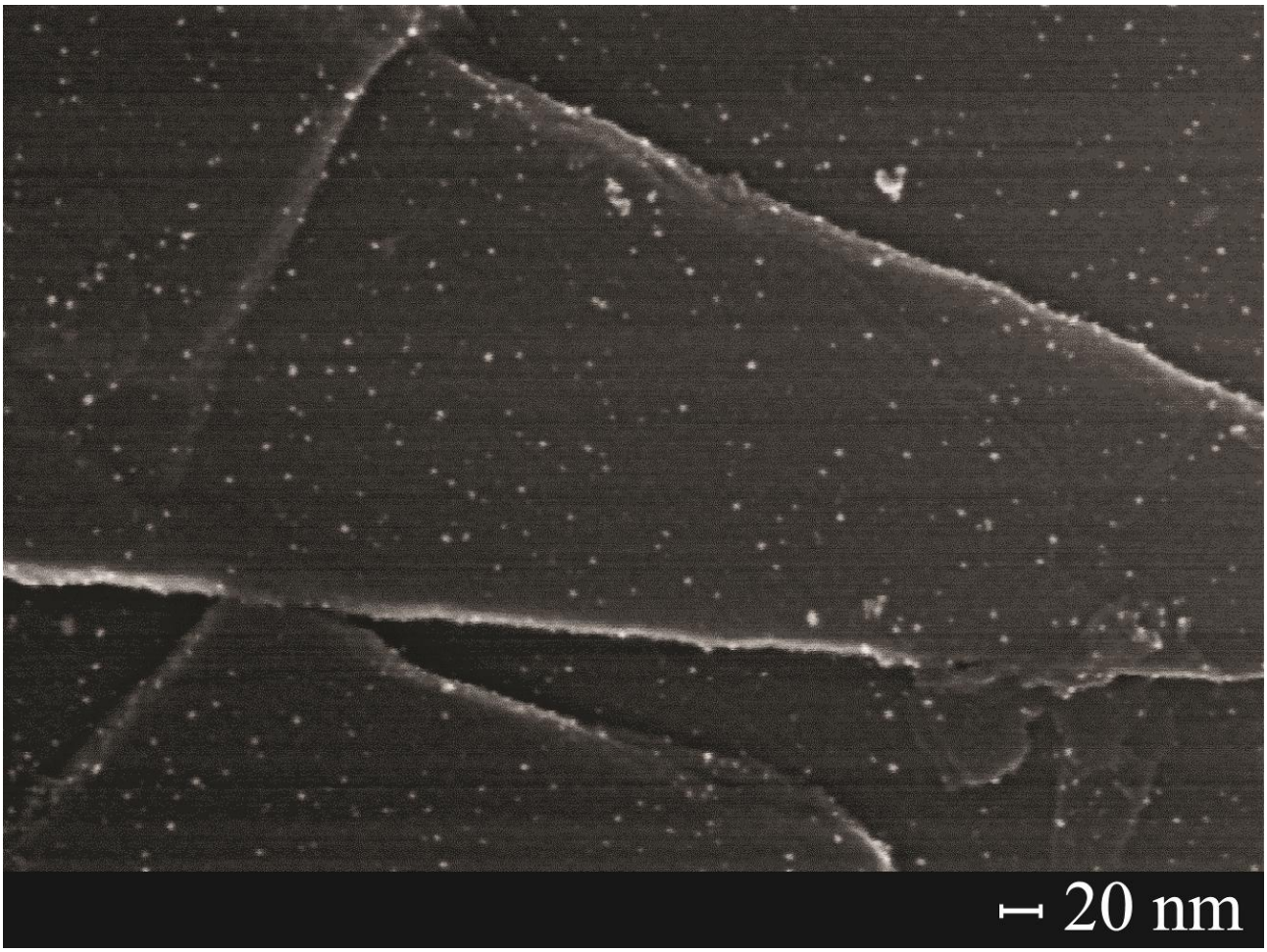

Figure S15. Enlarged image of the figure 6D.

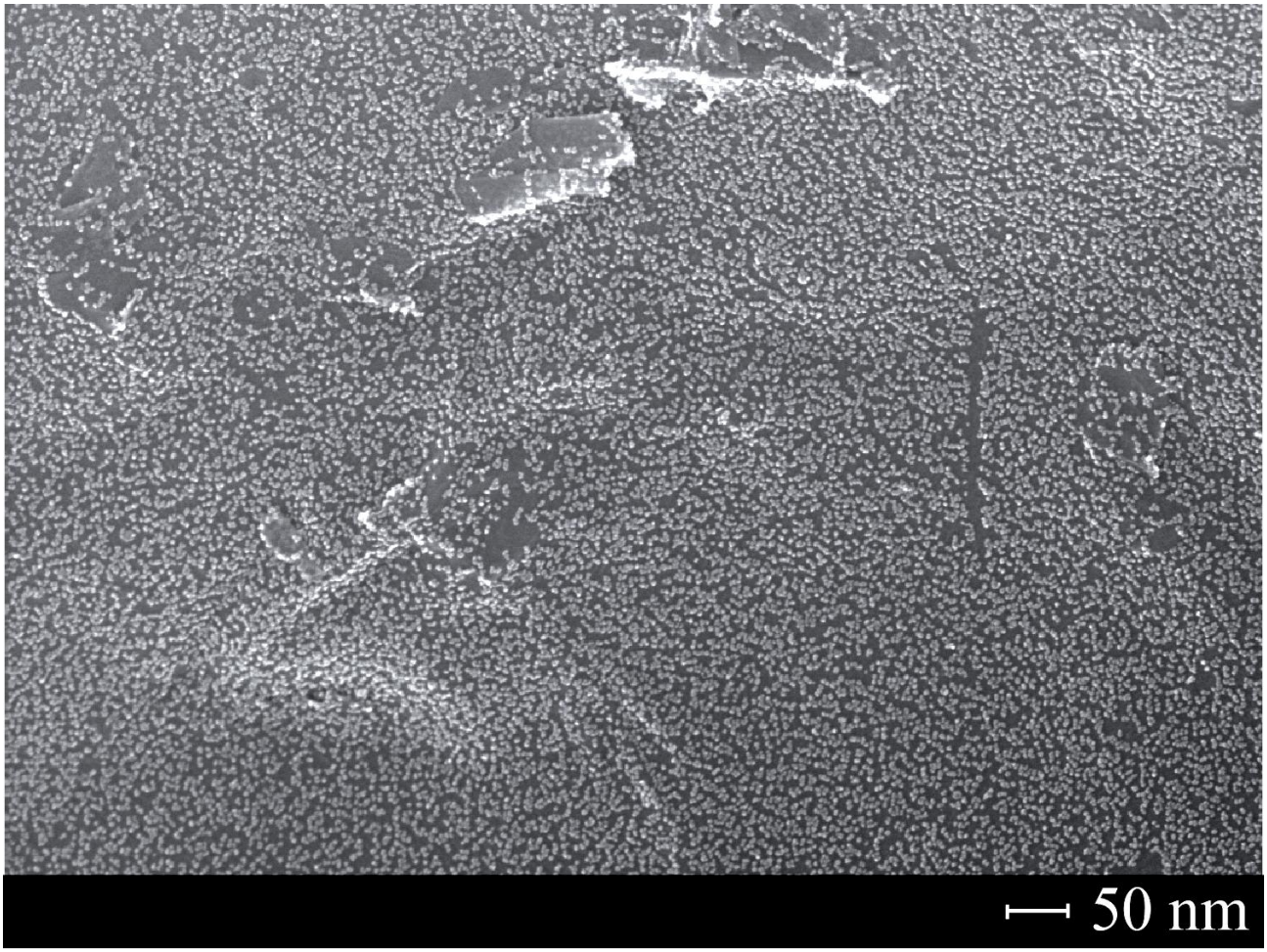

Figure S16. Image of palladium nanoparticles with uniform graphite surface coverage at high concentration of the metal precursor in solution.