Electric Supplementary Information

Bis(*β*-diketonato)- and Allyl-(*β*-diketonato)-Palladium(II) Complexes: Synthesis, Characterization and MOCVD Application

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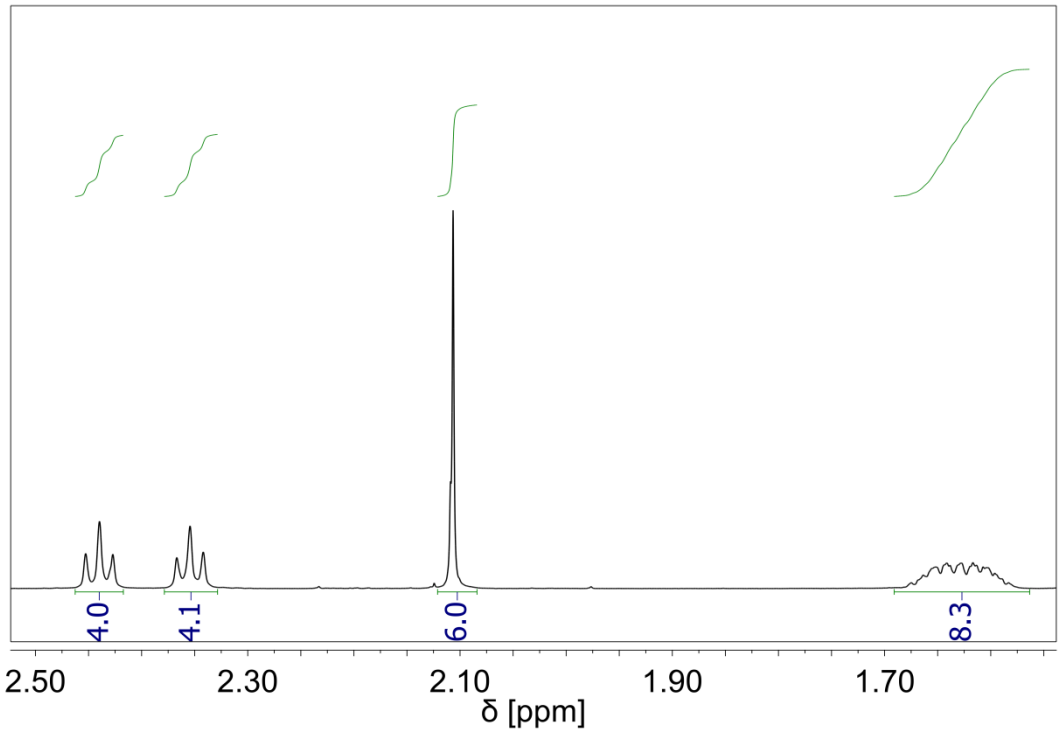
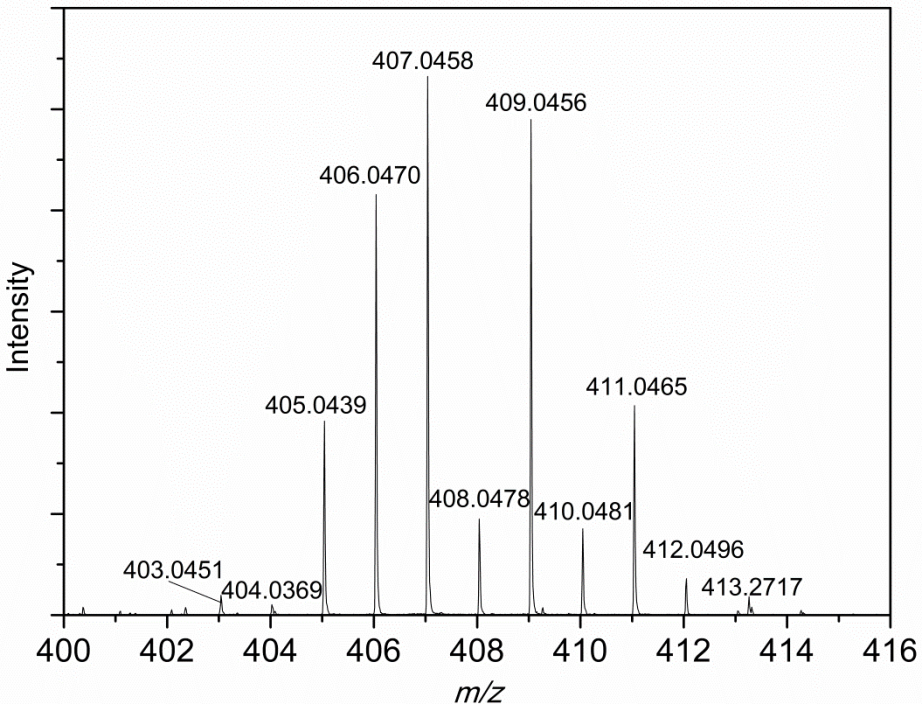
Content

^{1}H NMR spectrum of **8**



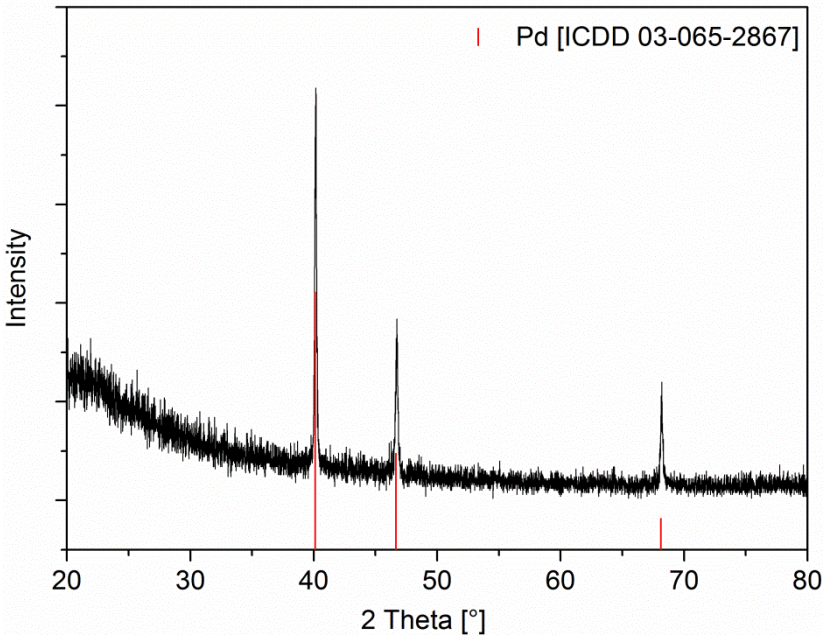
SI 1. ^{1}H NMR spectrum of **8** at 25 °C in chloroform.

ESI MS: Isotope pattern of $[M + Na]^+$ for **8**.

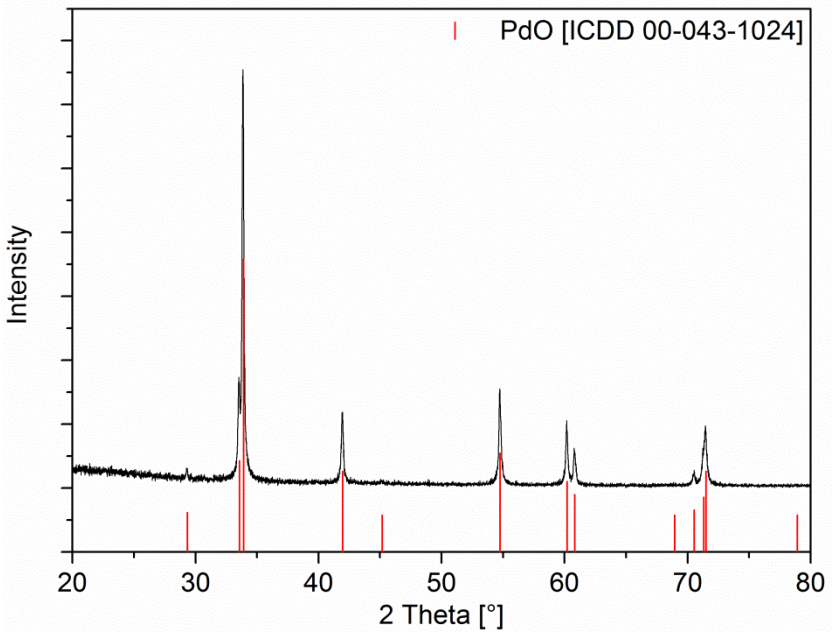


SI 2. Isotope pattern of the ion peak $[M + Na]^+$ from the ESI MS spectrum of **8**

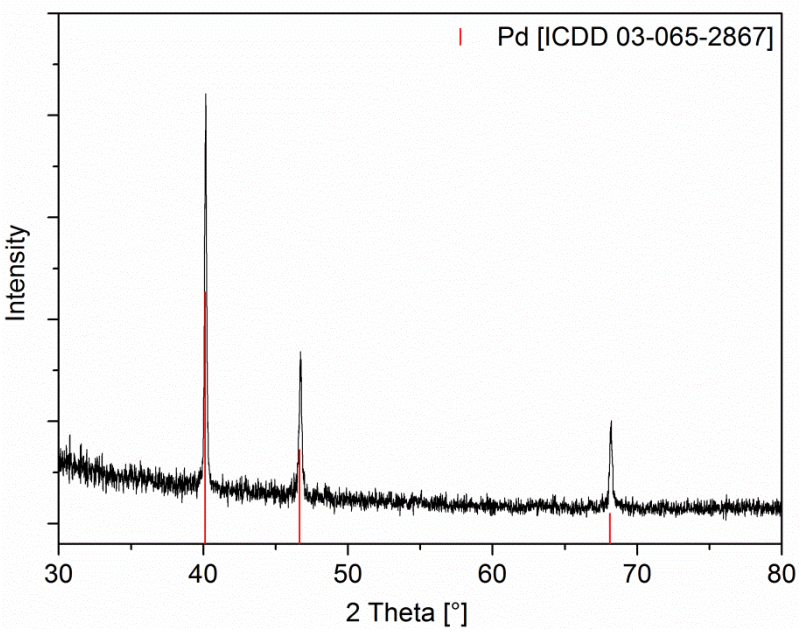
XRPD Pattern of the TG Residues



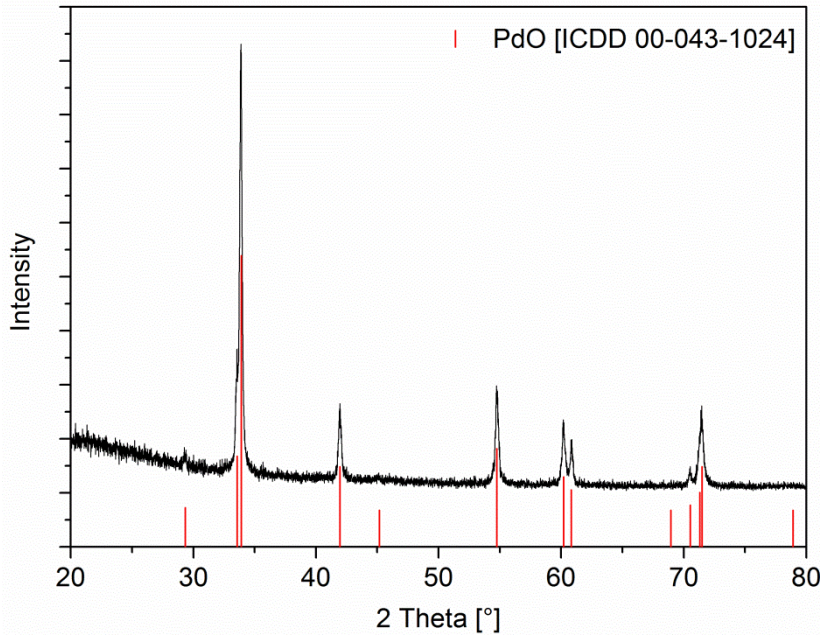
SI 3. XRPD pattern of the residue obtained by the TG of **7** under nitrogen (gas flow, 20 sccm; heating rate 10 K min^{-1}).



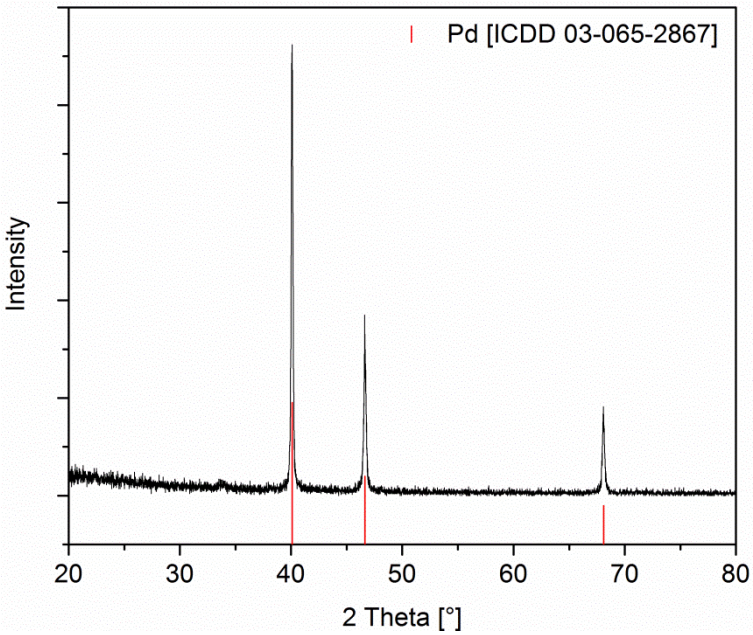
SI 4. XRPD pattern of the residue obtained by the TG of **7** under oxygen (gas flow, 20 sccm; heating rate 10 K min^{-1}).



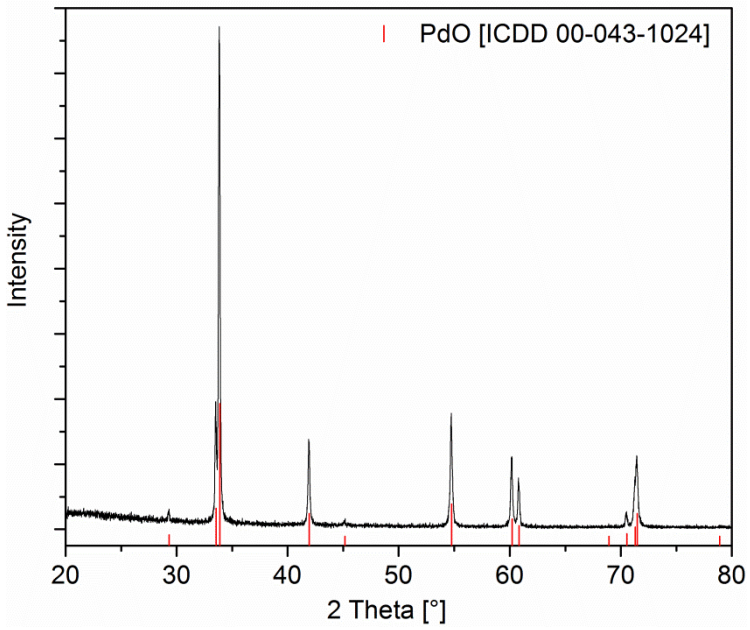
SI 5. XRPD pattern of the residue obtained by the TG of **8** under nitrogen (gas flow, 20 sccm; heating rate 10 K min^{-1}).



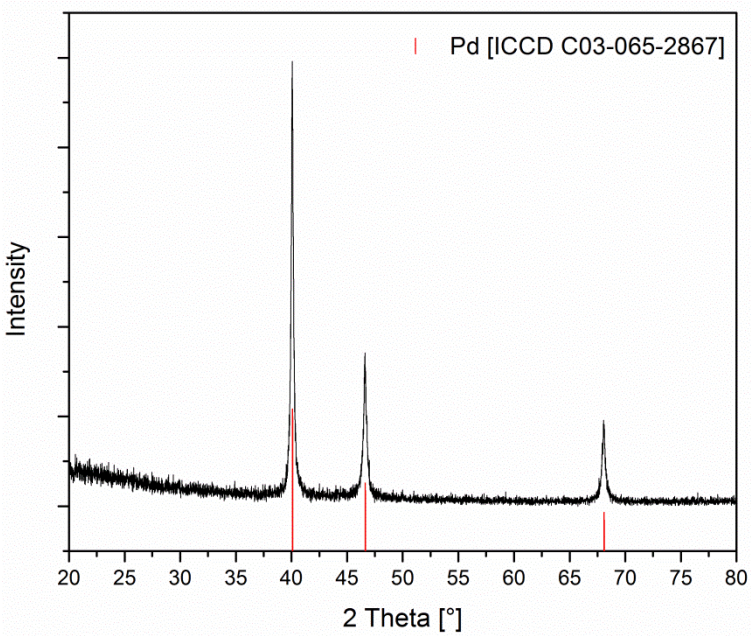
SI 6. XRPD pattern of the residue obtained by the TG of **8** under oxygen (gas flow, 20 sccm; heating rate 10 K min^{-1}).



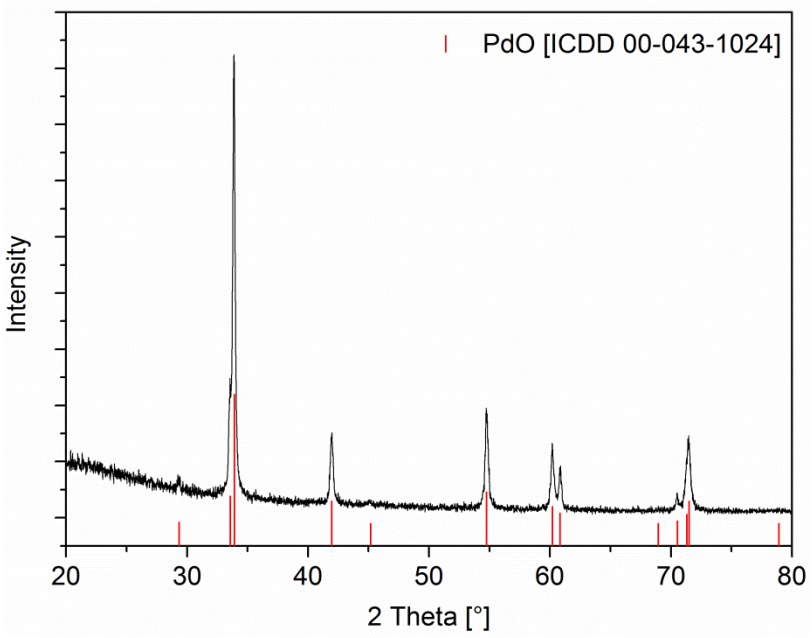
SI 7. XRPD pattern of the residue obtained by the TG of **11** under nitrogen (gas flow, 20 sccm; heating rate 10 K min^{-1}).



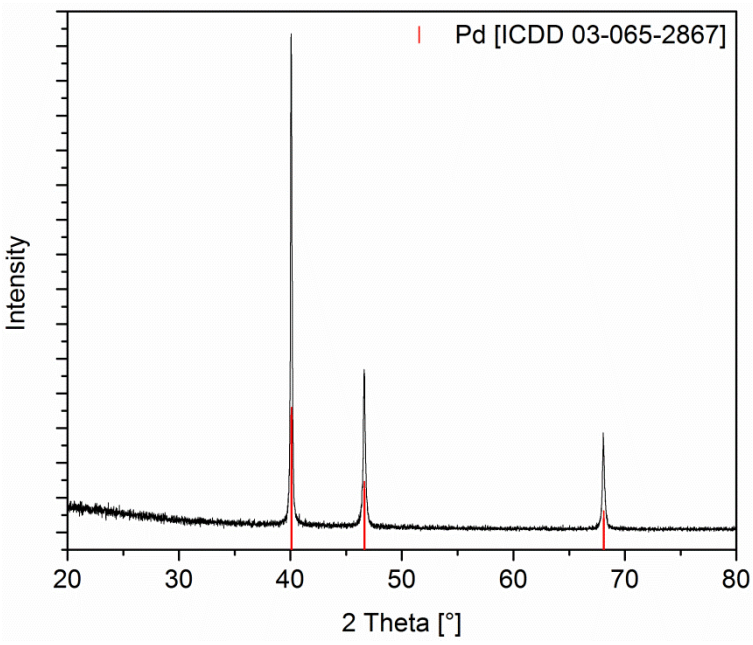
SI 8. XRPD pattern of the residue obtained by the TG of **11** under oxygen (gas flow, 20 sccm; heating rate 10 K min^{-1}).



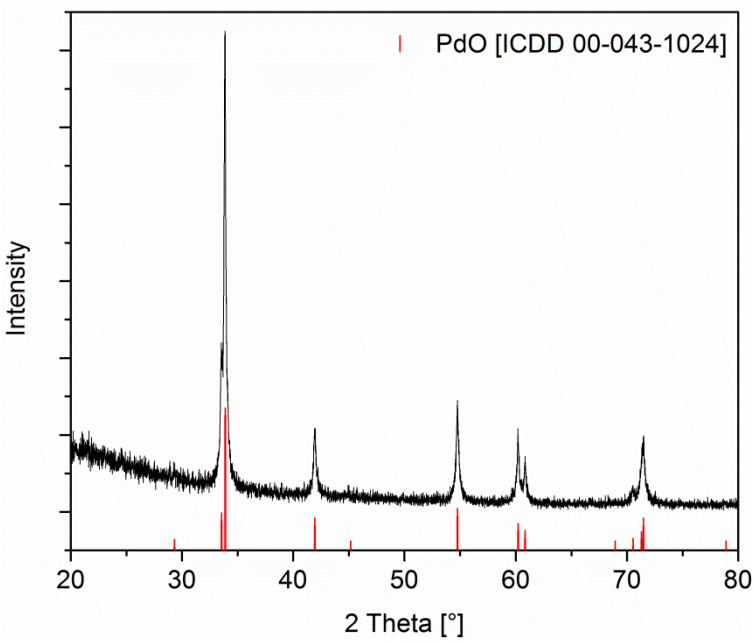
SI 9. XRPD pattern of the residue obtained by the TG of **12** under nitrogen (gas flow, 20 sccm; heating rate 10 K min^{-1}).



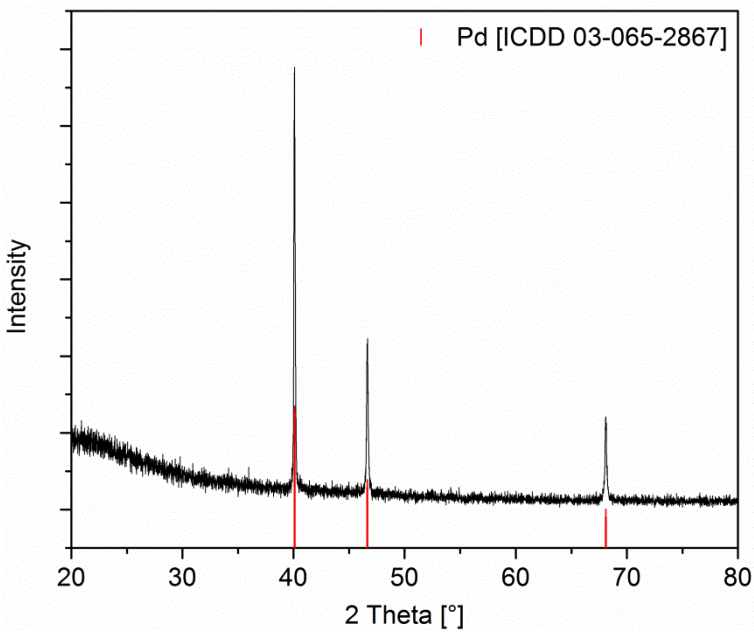
SI 10. XRPD pattern of the residue obtained by the TG of **12** under oxygen (gas flow, 20 sccm; heating rate 10 K min^{-1}).



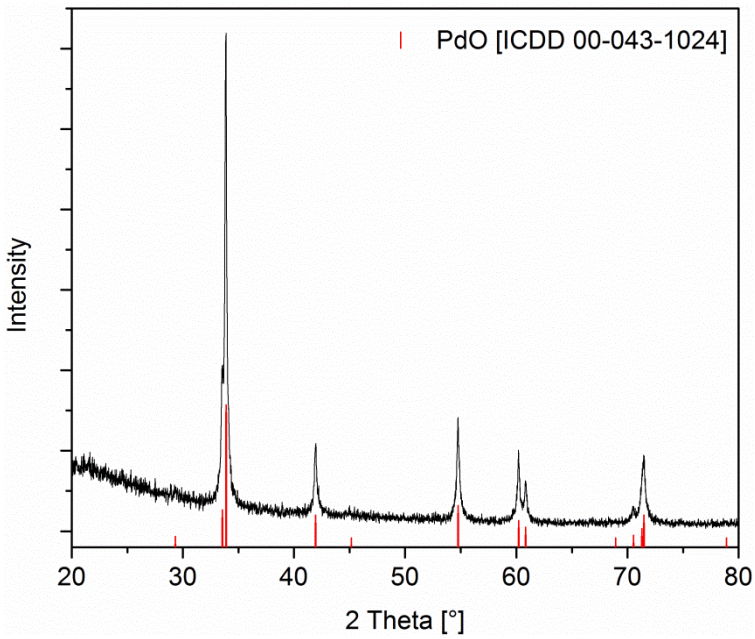
SI 11. XRPD pattern of the residue obtained by the TG of **13** under nitrogen (gas flow, 20 sccm; heating rate 10 K min^{-1}).



SI 12. XRPD pattern of the residue obtained by the TG of **13** under oxygen (gas flow, 20 sccm; heating rate 10 K min^{-1}).

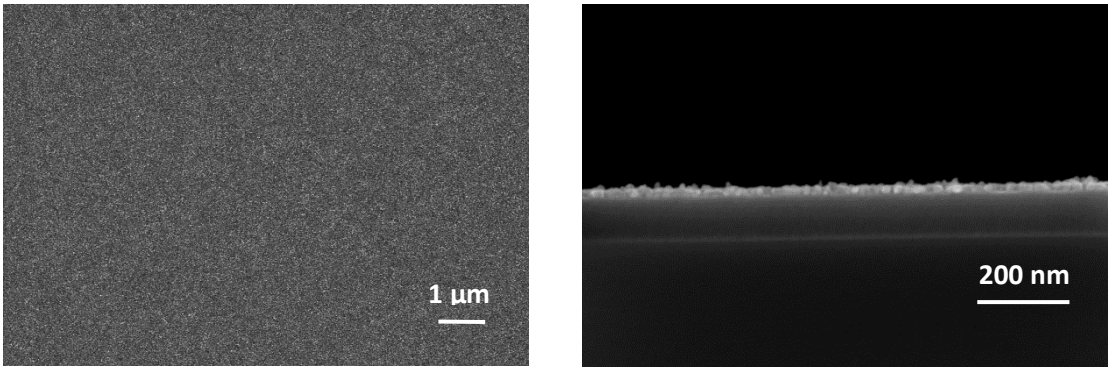


SI 13. XRPD pattern of the residue obtained by the TG of **14** under nitrogen (gas flow, 20 sccm; heating rate 10 K min^{-1}).

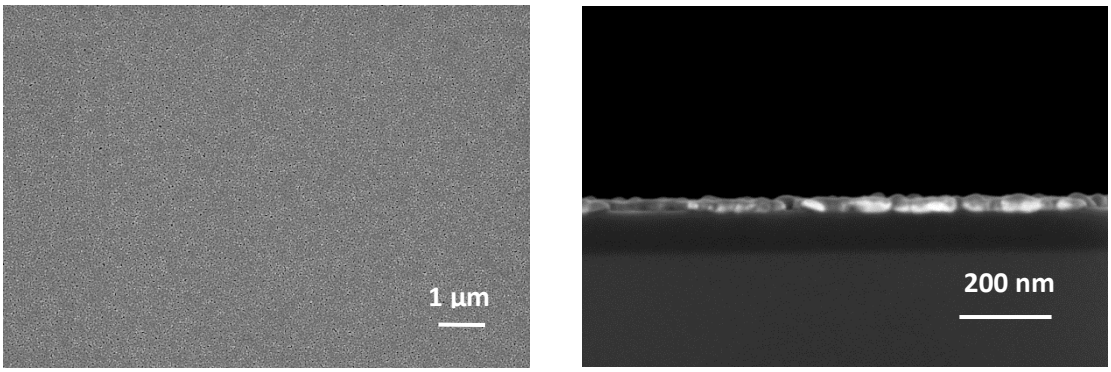


SI 14. XRPD pattern of the residue obtained by the TG of **14** under oxygen (gas flow, 20 sccm; heating rate 10 K min^{-1}).

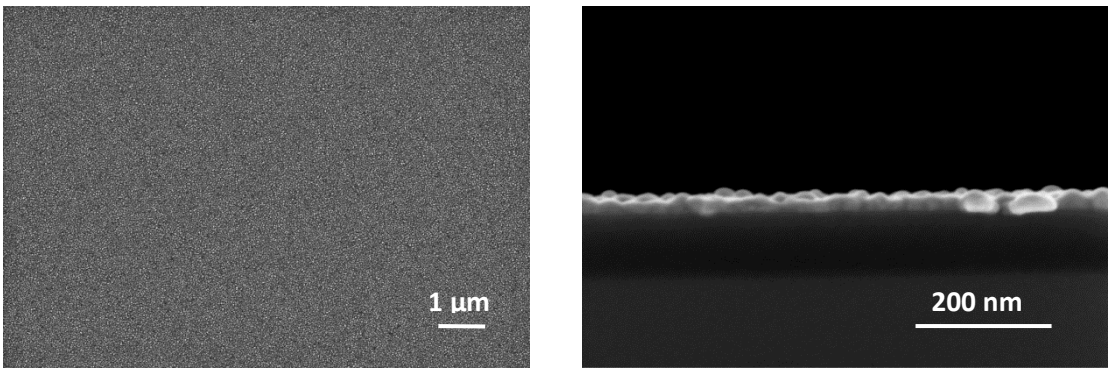
SEM Images



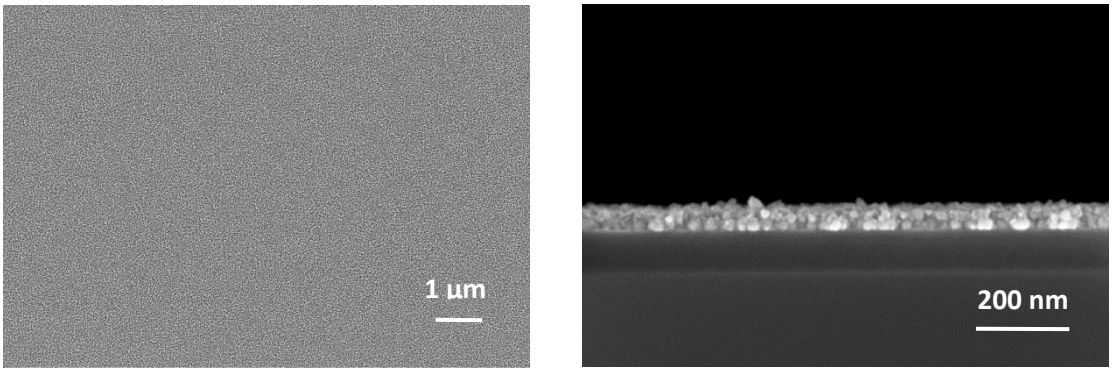
SI 15. Left: Layer obtained from the CVD(O_2) of **11**. Right: Cross-section image. Substrate temperature 380 °C, deposition time 15 min, nitrogen flow rate 40 sccm (carrier gas), oxygen flow rate 40 sccm, working pressure 0.8 mbar.



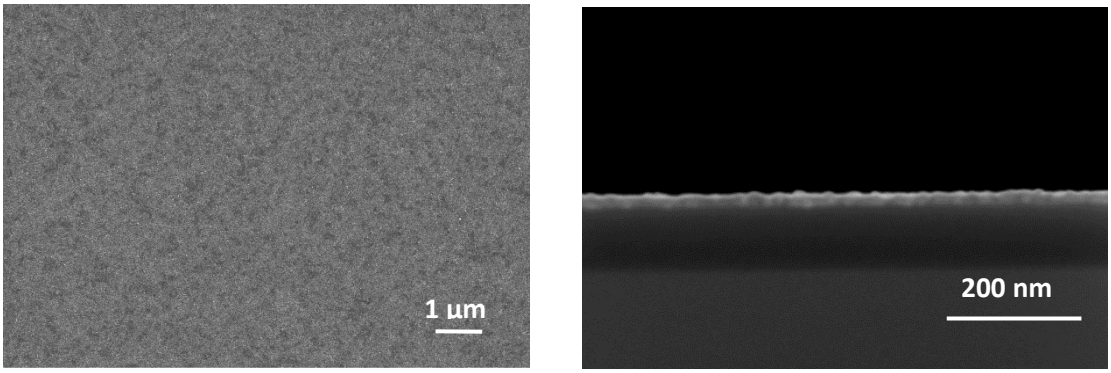
SI 16. Left: Layer obtained from the CVD(N_2/H_2) of **11**. Right: Cross-section image. Substrate temperature 350 °C, deposition time 15 min, nitrogen flow rate 40 sccm (carrier gas), forming gas 40 sccm, working pressure 0.8 mbar.



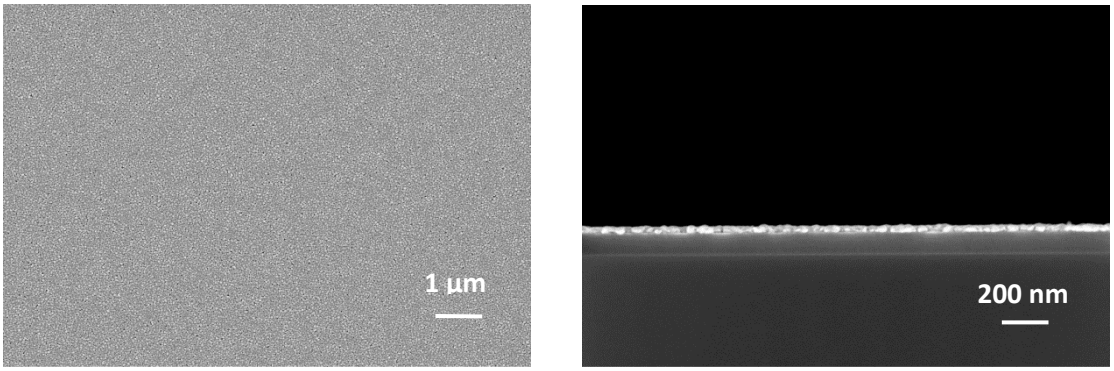
SI 17. Left: Layer obtained from the CVD(O_2) of **12**. Right: Cross-section image. Substrate temperature 380 °C, deposition time 15 min, nitrogen flow rate 40 sccm (carrier gas), oxygen flow rate 40 sccm, working pressure 0.8 mbar.



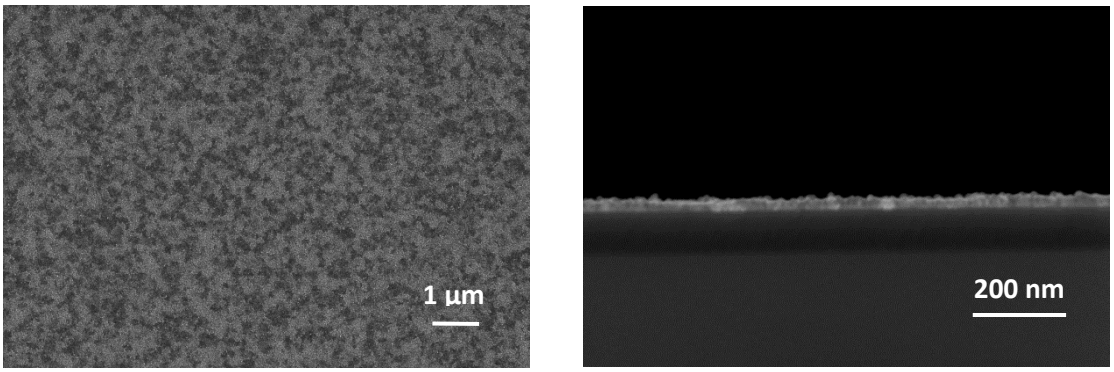
SI 18. Left: Layer obtained from the CVD(N_2/H_2) of **12**. Right: Cross-section image. Substrate temperature 350 °C, deposition time 15 min, nitrogen flow rate 40 sccm (carrier gas), forming gas 40 sccm, working pressure 0.8 mbar.



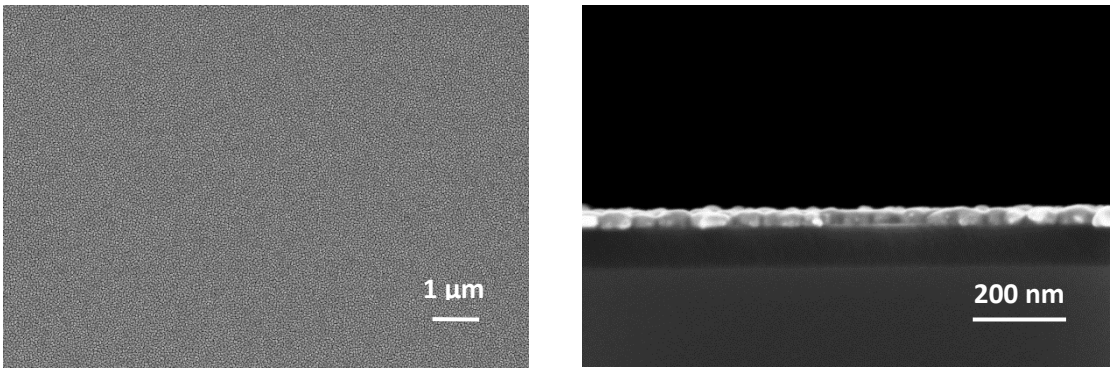
SI 19. Left: Layer obtained from the CVD(O_2) of **13**. Right: Cross-section image. Substrate temperature 380 °C, deposition time 15 min, nitrogen flow rate 40 sccm (carrier gas), oxygen flow rate 40 sccm, working pressure 0.8 mbar.



SI 20. Left: Layer obtained from the CVD(N_2/H_2) of **13**. Right: Cross-section image. Substrate temperature 350 °C, deposition time 15 min, nitrogen flow rate 40 sccm (carrier gas), forming gas 40 sccm, working pressure 0.8 mbar.

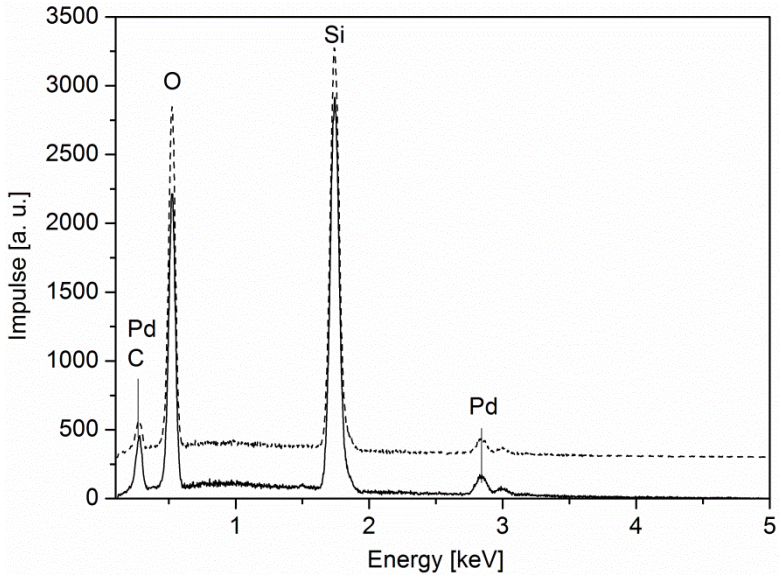


SI 21. Left: Layer obtained from the CVD(O_2) of **14**. Right: Cross-section image. Substrate temperature 380 °C, deposition time 15 min, nitrogen flow rate 40 sccm (carrier gas), oxygen flow rate 40 sccm, working pressure 0.8 mbar.

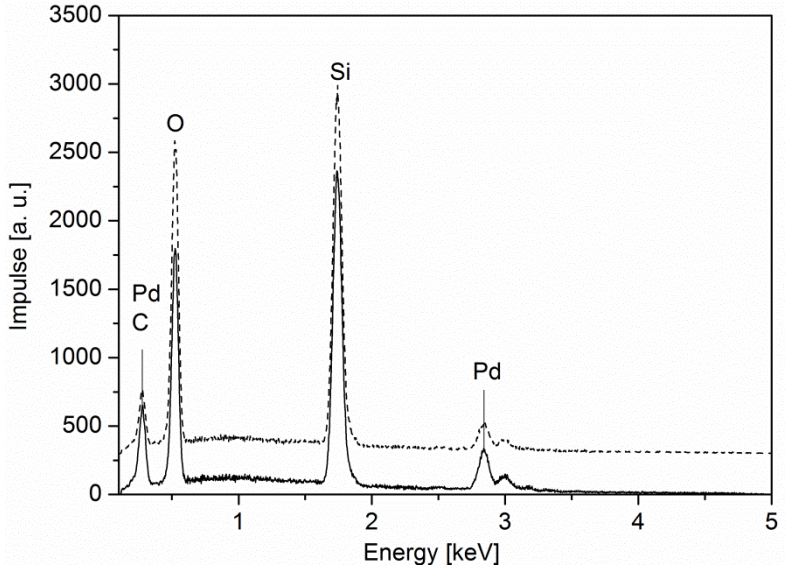


SI 22. Left: Layer obtained from the CVD(N_2/H_2) of **14**. Right: Cross-section image. Substrate temperature 350 °C, deposition time 15 min, nitrogen flow rate 40 sccm (carrier gas), forming gas 40 sccm, working pressure 0.8 mbar.

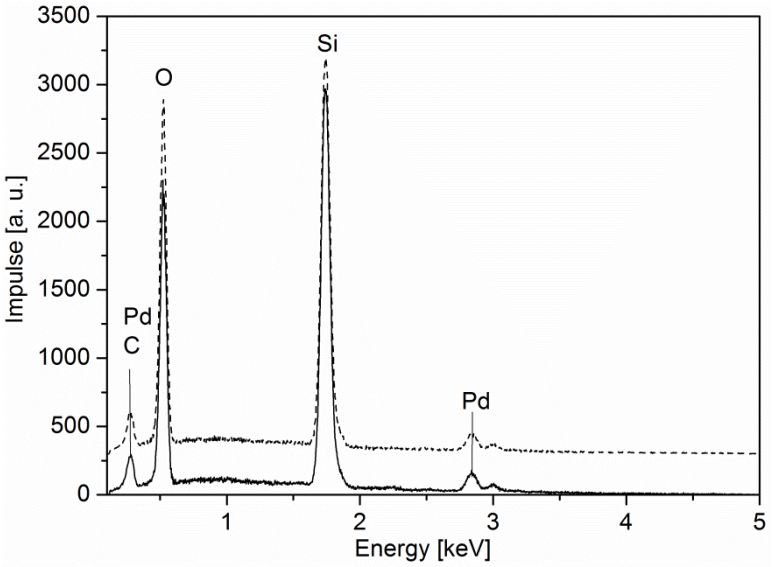
EDX Spectra



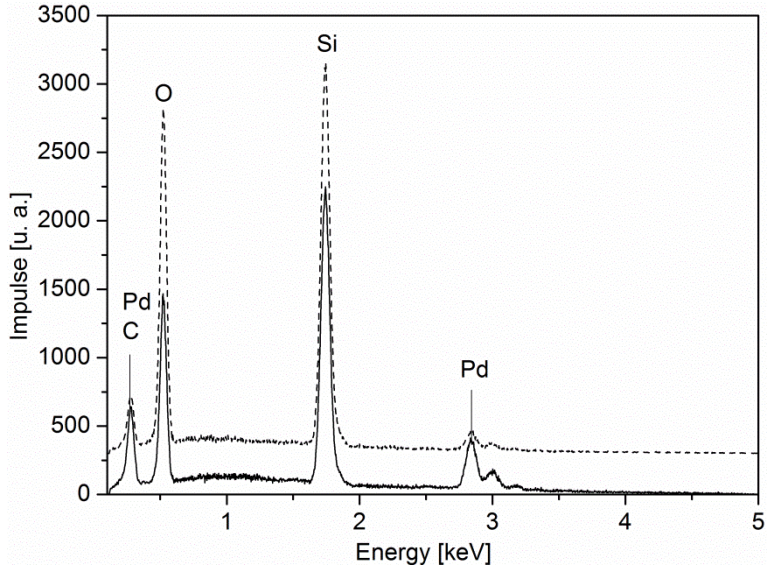
SI 23. EDX spectra of the film obtained from **11** by CVD(O_2) (dotted, oxygen flow rate 40 sccm, substrate temperature 380 °C) and CVD(N_2/H_2) (solid, forming gas flow rate 40 sccm, substrate temperature 350 °C) for comparison.



SI 24. EDX spectra of the film obtained from **12** by CVD(O_2) (dotted, oxygen flow rate 40 sccm, substrate temperature 380 °C) and CVD(N_2/H_2) (solid, forming gas flow rate 40 sccm, substrate temperature 350 °C) for comparison.

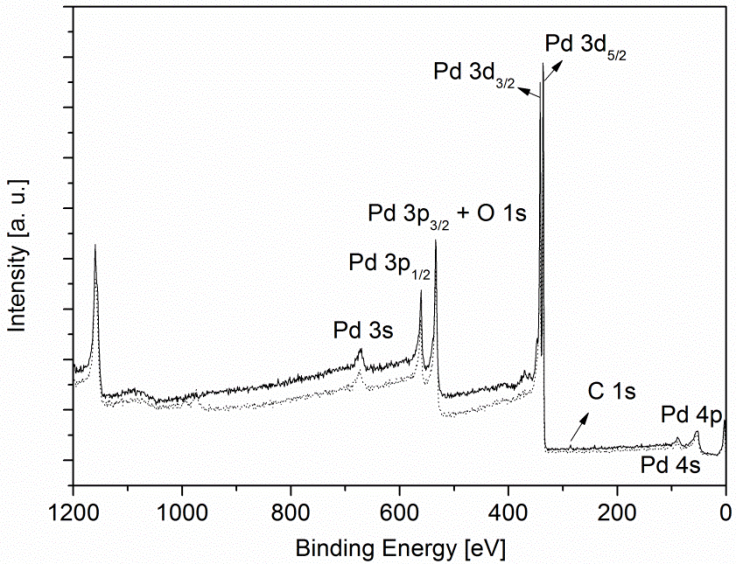


SI 25. EDX spectra of the film obtained from **13** by CVD(O_2) (dotted, oxygen flow rate 40 sccm, substrate temperature 380 °C) and CVD(N_2/H_2) (solid, forming gas flow rate 40 sccm, substrate temperature 350 °C) for comparison.

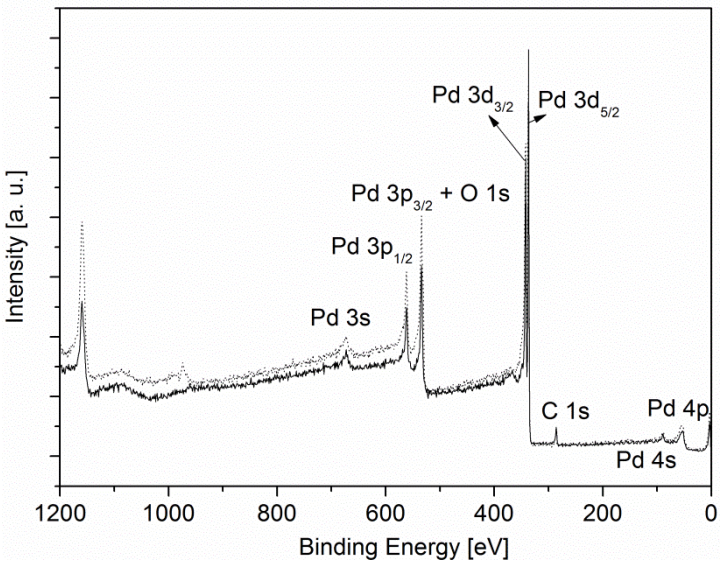


SI 26. EDX spectra of the film obtained from **14** by CVD(O_2) (dotted, oxygen flow rate 40 sccm, substrate temperature 380 °C) and CVD(N_2/H_2) (solid, forming gas flow rate 40 sccm, substrate temperature 350 °C) for comparison.

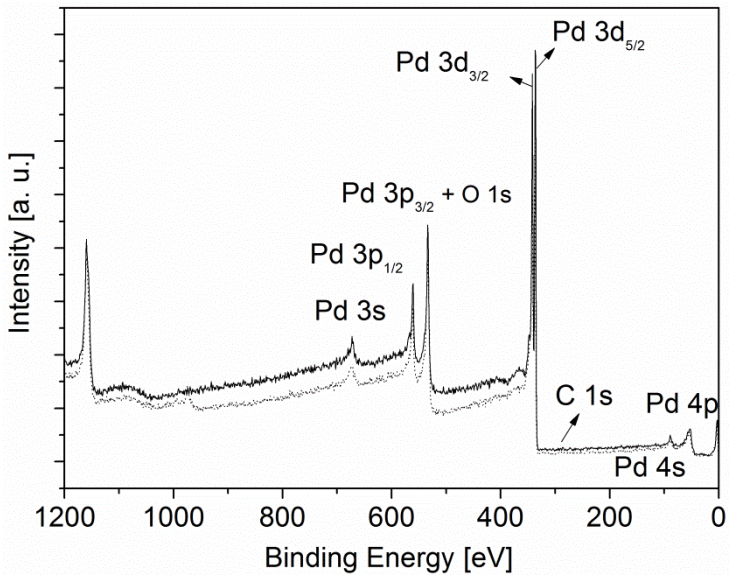
XPS Spectra



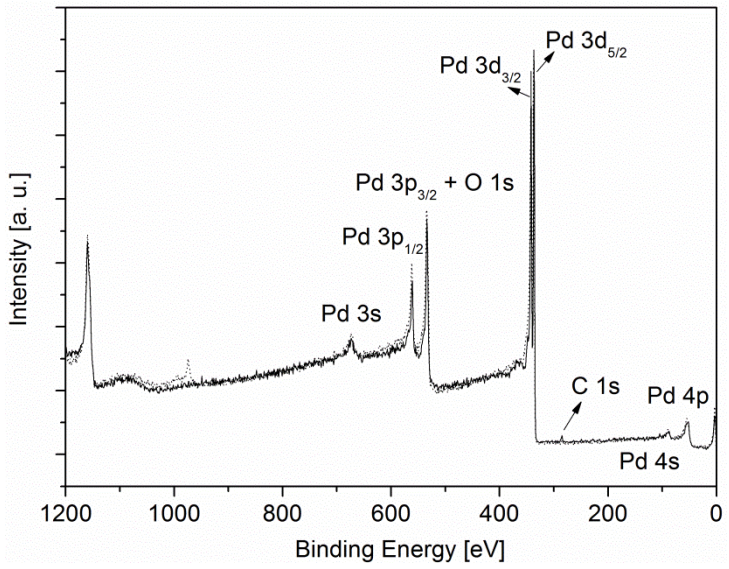
SI 27. *Ex-situ* XPS spectra of the film obtained from **11** by CVD(O_2) (dotted, oxygen flow rate 40 sccm, substrate temperature 380 °C) and CVD(N_2/H_2) (solid, forming gas flow rate 40 sccm, substrate temperature 350 °C) for comparison.



SI 28. *Ex-situ* XPS spectra of the film obtained from **12** by CVD(O_2) (dotted, oxygen flow rate 40 sccm, substrate temperature 380 °C) and CVD(N_2/H_2) (solid, forming gas flow rate 40 sccm, substrate temperature 350 °C) for comparison.



SI 29. *Ex-situ* XPS spectra of the film obtained from **13** by CVD(O_2) (dotted, oxygen flow rate 40 sccm, substrate temperature 380 °C) and CVD(N_2/H_2) (solid, forming gas flow rate 40 sccm, substrate temperature 350 °C) for comparison.



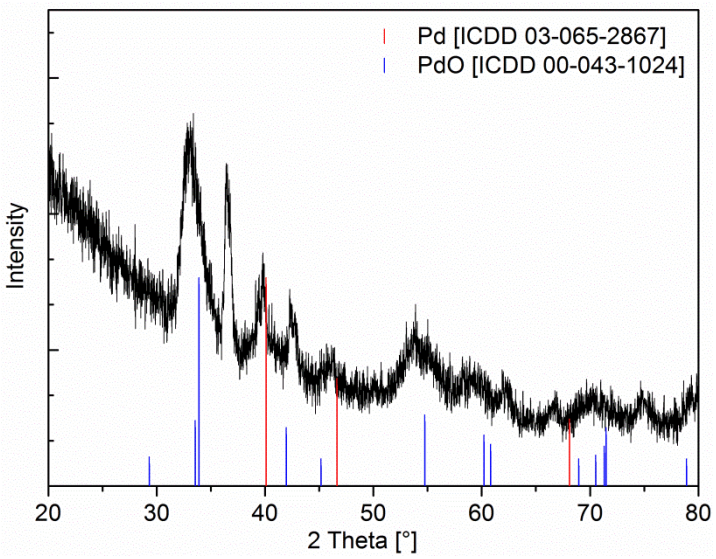
SI 30. *Ex-situ* XPS spectra of the film obtained from **14** by CVD(O_2) (dotted, oxygen flow rate 40 sccm, substrate temperature 380 °C) and CVD(N_2/H_2) (solid, forming gas flow rate 40 sccm, substrate temperature 350 °C) for comparison.

XPS Fitting Parameters

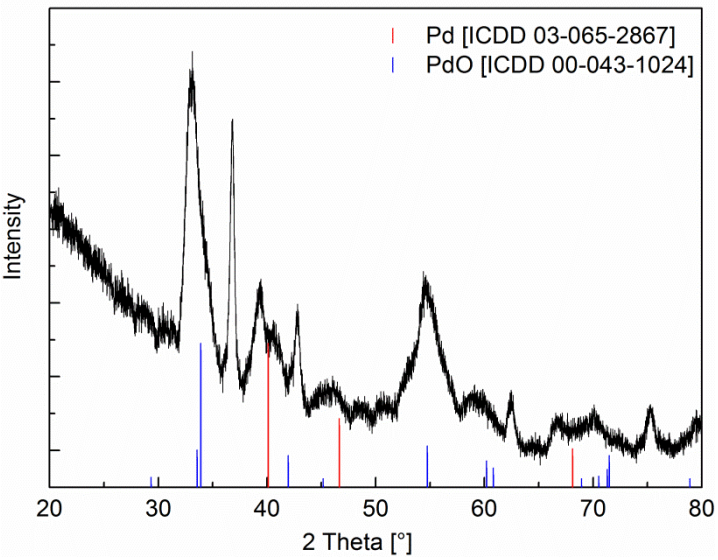
SI 31. Fitting parameters of the Pd $3p_{3/2}$ and Pd $3p_{1/2}$ peaks obtained from PVD and CVD processes.

	PVD		CVD		
	A	B	C	D	E
Peak	Pd $3p_{3/2}$	Pd $3p_{1/2}$	Pd $3p_{3/2}$ (plasmon loss)	Pd $p3_{1/2}$ (plasmon loss)	O 1s
Area restrictions	2 x B	-	-	-	-
FWHM restictions [eV]	≤ 5.0 eV	≤ 5.0 eV	≤ 5.0 eV	≤ 5.0 eV	≤ 2.5 eV
Binding energy [eV]	531.5 - 534.0	A + 28.8	A + 5.3	A + 33.1	559.0 - 531.0
Peak shape	GL(70)	GL(90)	GL(30)T(2)	GL(30)T(2)	GL(30)

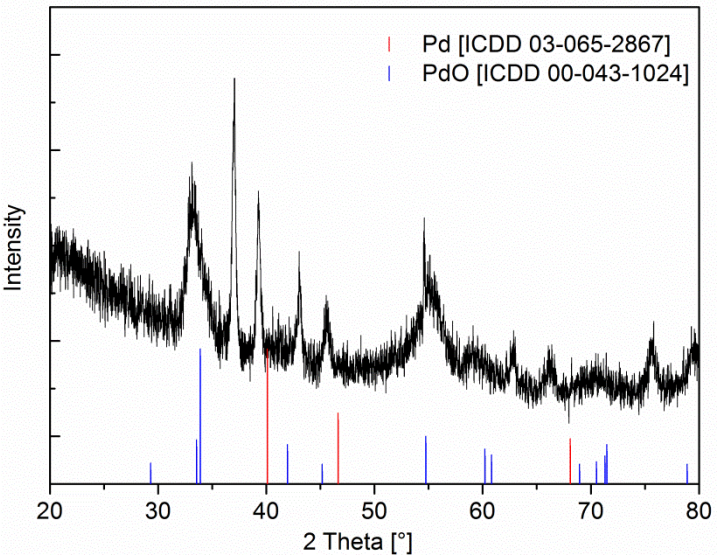
XRPD Pattern of the Deposited Films



SI 32. XRPD pattern obtained from the layer formed by **11** CVD(O_2).



SI 33. XRPD pattern obtained from the layer formed by **12** CVD(O_2).



SI 34. XRPD pattern obtained from the layer formed by **14** CVD(O_2).