SUPPORTING INFORMATION

Investigation of the catalytic performance of Pd/CNFs for hydrogen evolution from additive-free formic acid decomposition

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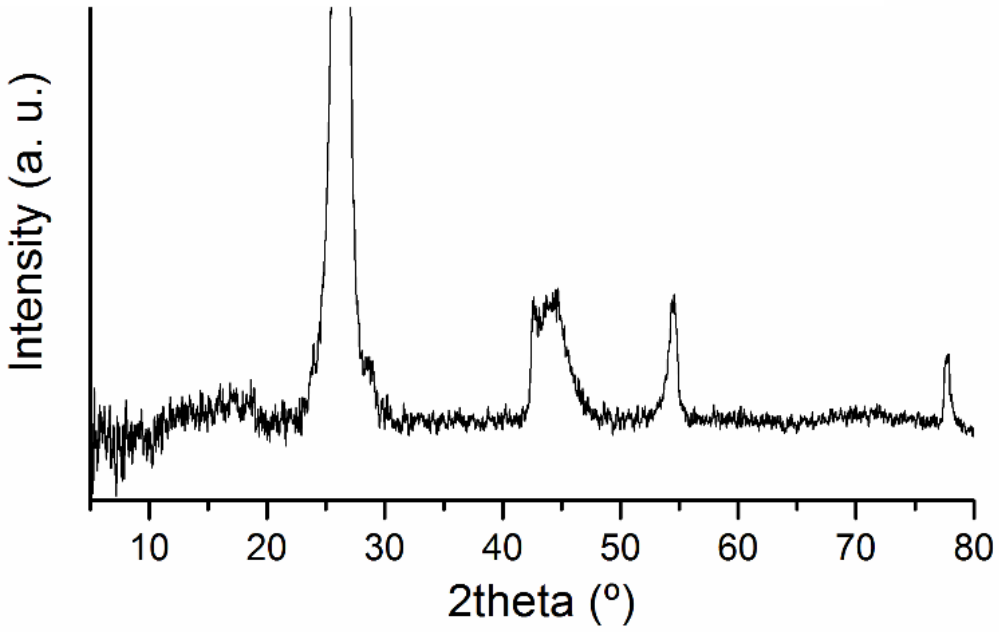

Fig. S1 XRD pattern of the CNF support.

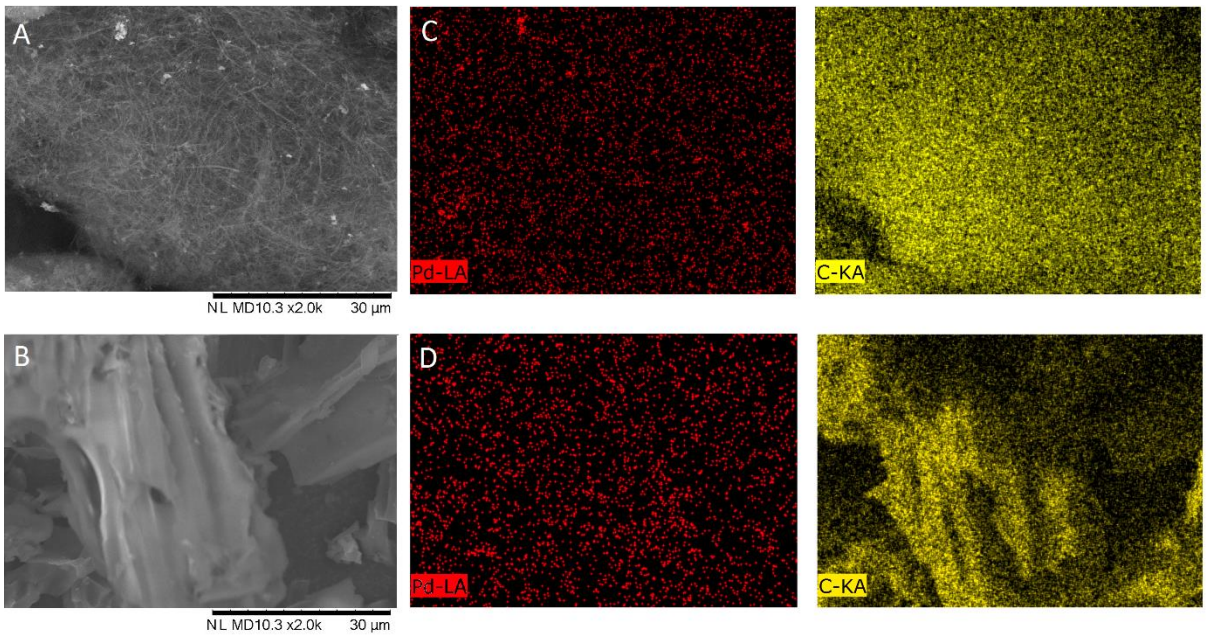

Fig. S2 (A) SEM image of Pd_{IMP}/CNF, (B) SEM image of Pd_{SI}/AC, (C) Mapping-EDX images of Pd_{IMP}/CNF (D) Mapping-EDX images of Pd_{SI}/AC.

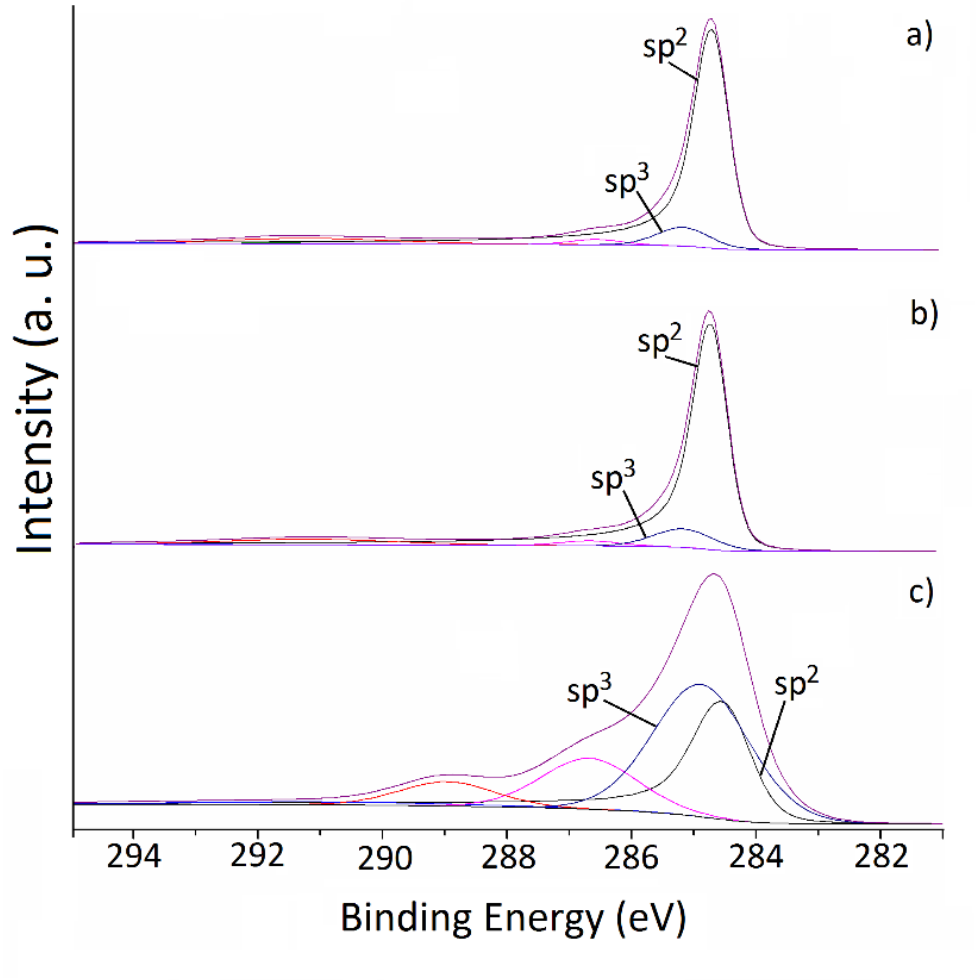

Figure S3. XPS spectra of (a) Pd_{IMP}/CNF, (b) Pd_{SI}/CNF and (c) Pd_{SI}/AC in the binding energy region of 281–295 eV corresponding to C1s.

Table S1 Atomic content of sp^2 and sp^3 carbon and ratio sp^2/sp^3 from XPS for the catalysts subjected to different temperature treatments.

Catalyst	C sp^2 (%)	C sp^3 (%)	sp^2/sp^3
Pd_{IMP}/CNF	82.10	7.50	10.95
Pd_{SI}/CNF	81.87	8.11	10.09
Pd_{SI}/AC	31.87	41.48	0.77

Table S2 BET surface areas for the as-synthesised catalysts and supports.

Catalyst	Support	IMP	SI
Pd/CNF	34	37	36
Pd/AC	64	-	32

Calculation of the number of surface exposed atoms

Calculations of the number of exposed surface atoms were performed by assuming that all the nanoparticles had cub-octahedral morphology with cubic close-packed structure in this size range, the model of full-shell nanoparticles was adopted.[1] The total number of the Au atoms in the cluster for a given cluster size can be calculated using the following equation (1):

$d_{sph} = 1.105\ d_{at} N_T^{1/3}$ (1)

Where d_{sph} is the mean diameter of the Au particles obtained from TEM analysis and d_{at} is the atom diameter of Pd, 0.274 nm. The number of surface atoms (Ns) and n can be calculated from equations (2) and (3), based on the values of NT:

$N_T = (10n^3 - 15n^2 + 11n - 3)/3$ (2)

$N_s = 10n^2 - 20n + 12$ (3)

Calculation of TOF based on the surface atoms

The TOF based on the surface atoms can then be calculated as follows:[2]

% of fraction of atoms lying at the surface:

$A = (Ns/NT)\ x100$

TOF based on Ns= TOF(calculated for bulk gold using the nominal weight)/A

References

1. K. Mori, T. Hara, T. Mizugaki, K. Ebitani, K. Kaneda, JACS 126 (2004) 10657-10666.
2. M. Comotti, C. Della Pina, R. Matarrese, M. Rossi, Angew. Chem. Int. Ed. 43 (2004) 5812-5815.