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Enhanced stability of sub-nanometric Iridium decorated graphitic carbon nitride for H_2 production upon hydrous hydrazine decomposition

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Supporting Information

Table S1 Fitting models employed for the high-resolution x-ray photoelectron spectroscopy analysis of the samples.

Samples	Ir/graphite		Ir/GCN		References
	Contribution	BE / eV	Contribution	BE / eV	
C 1s	C sp^2	284.3	C-N=C	285.4	64,66
	C sp^3	285.1	C=C	288.7	
	C-O	285.6	/	/	
	C=O	286.2	/	/	
N 1s	N_2H_x	400.2	C=N	398.5	64,65,98
	N_2H_x	401.5	C=N-H	399.9	
	NH_x	398.6	qN	400.9	
	/	/	NO_x	404.1	
Ir 4f	Ir^0	60.7	Ir^0	60.7	67
	Ir^{IV}	61.7	Ir^{IV}	61.7	
	$Ir^{IV\text{-}OH}$	62.3	$Ir^{IV\text{-}OH}$	62.3	

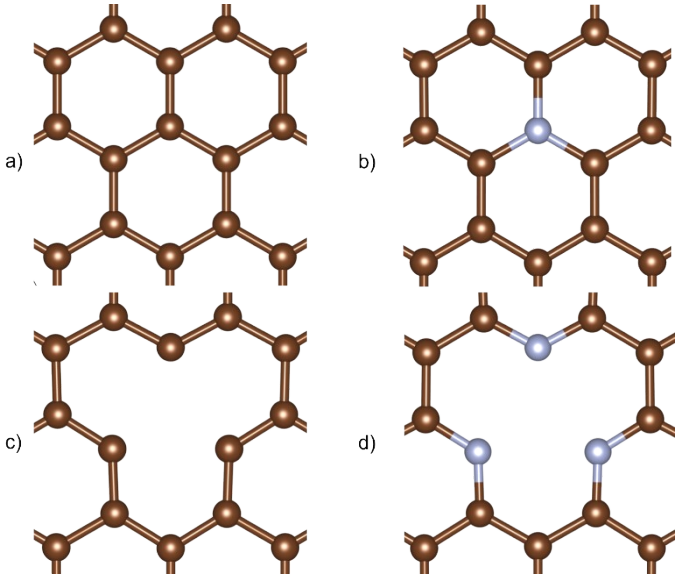

Figure S1. Top view of the optimised slabs employed for the Genetic Algorithm (GA) runs. a) pristine graphene (PG). b) graphitic N (gN), c) Single Vacancy (SV) and d) tripe pyridinic N (3pN). Carbon and nitrogen atoms are coloured brown and blue respectively.

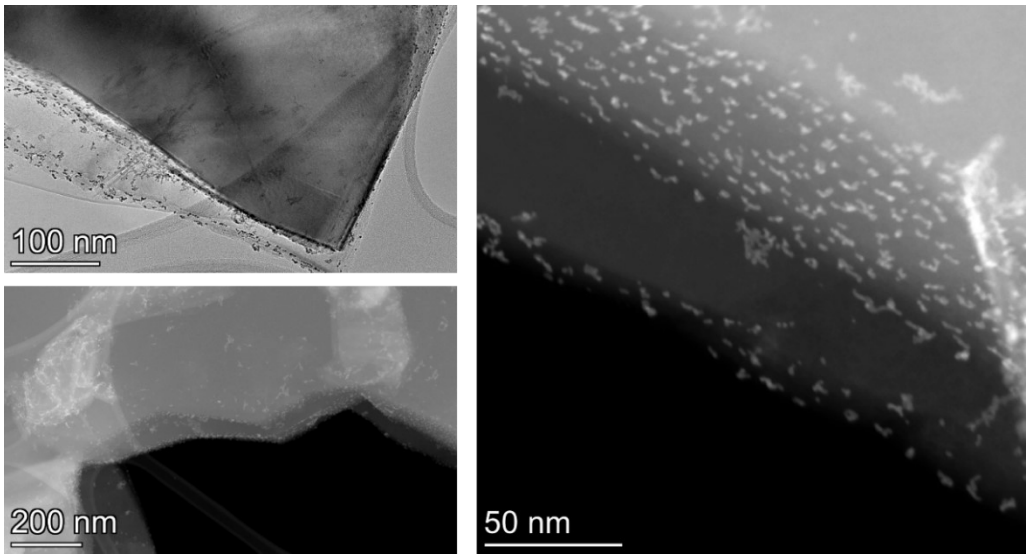

Figure S2. HR-TEM/STEM-HAADF images of Ir/graphite showing the preferential anchoring at grain boundaries.

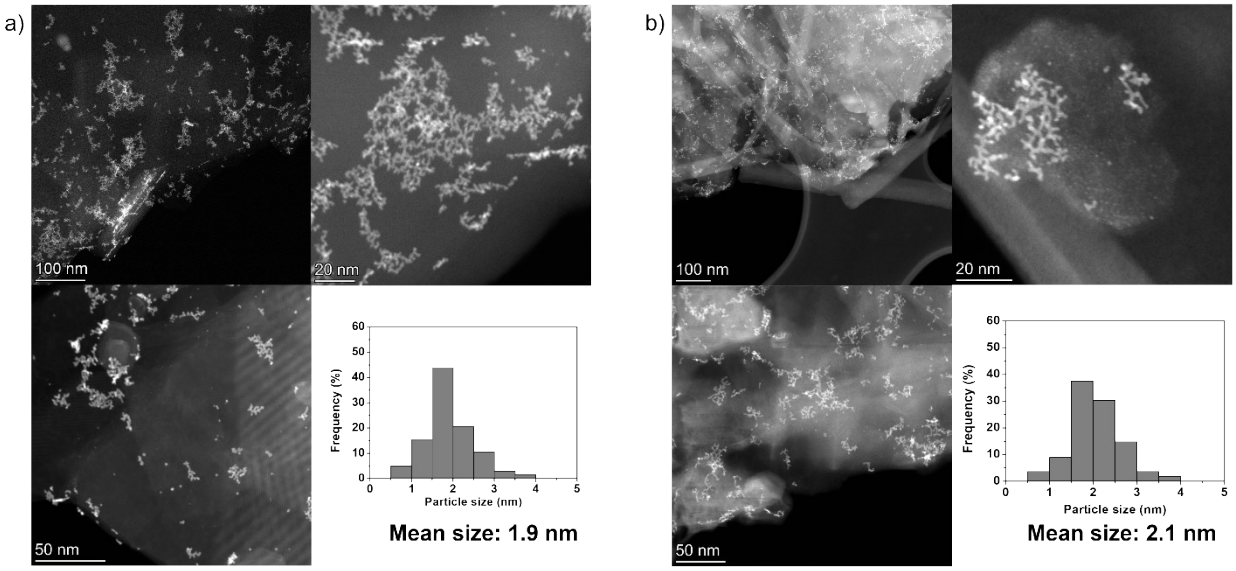

Figure S3. STEM-HAADF images of Ir/graphite a) fresh and b) after 5 repeated reaction cycles.

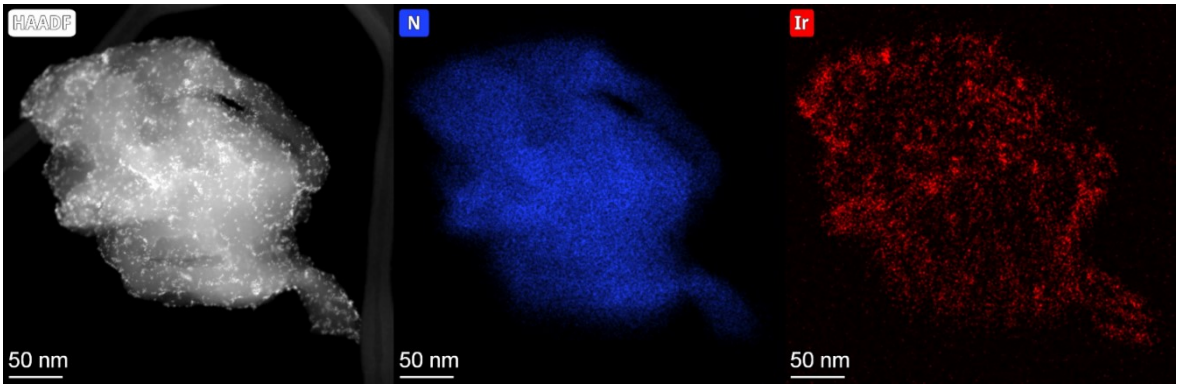

Figure S4. HAADF-STEM image, N and Ir maps of fresh Ir/GCN catalyst.

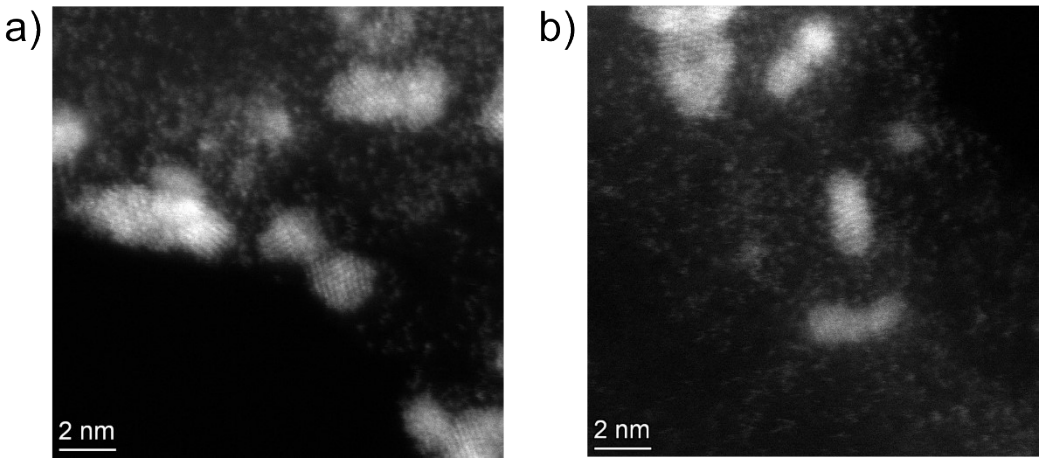

Figure S5. High resolution HAADF-STEM images of Ir/GCN, a) fresh and b) after 5 runs.

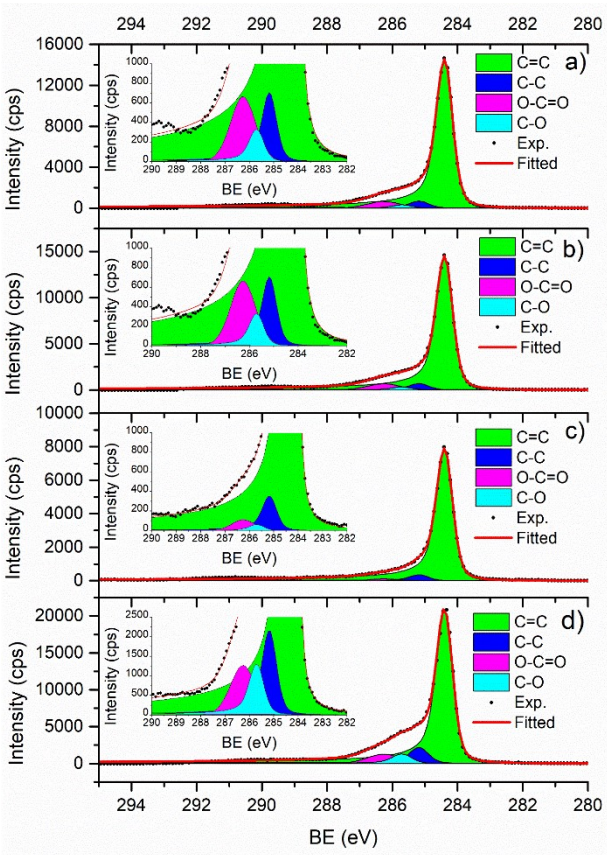

Figure S6. High resolution C 1s region for graphite samples: support a), Ir/graphite b) fresh, c) 1 run and d) 5 run.

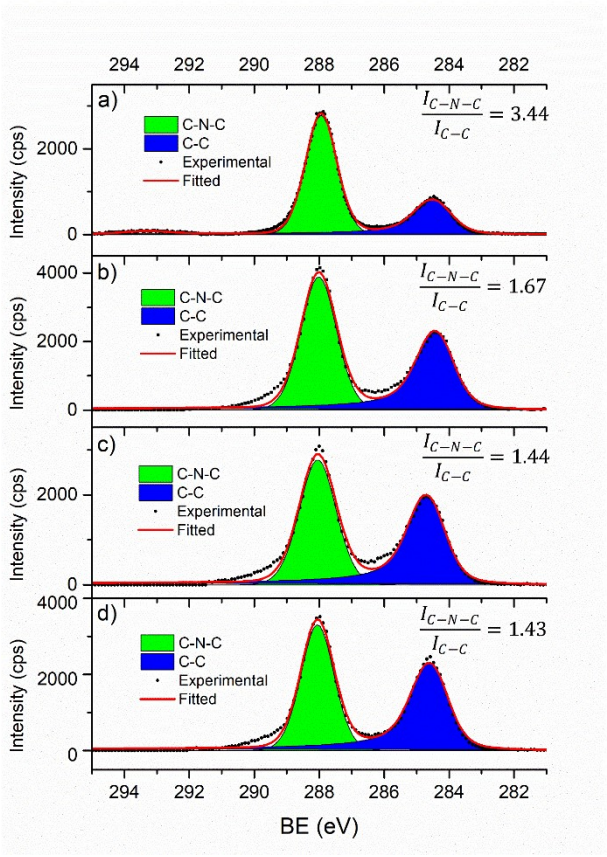

Figure S7. High resolution C 1s region for GCN samples: a) support, Ir/ GCN b) fresh, c) 1 run and d) 5 run.

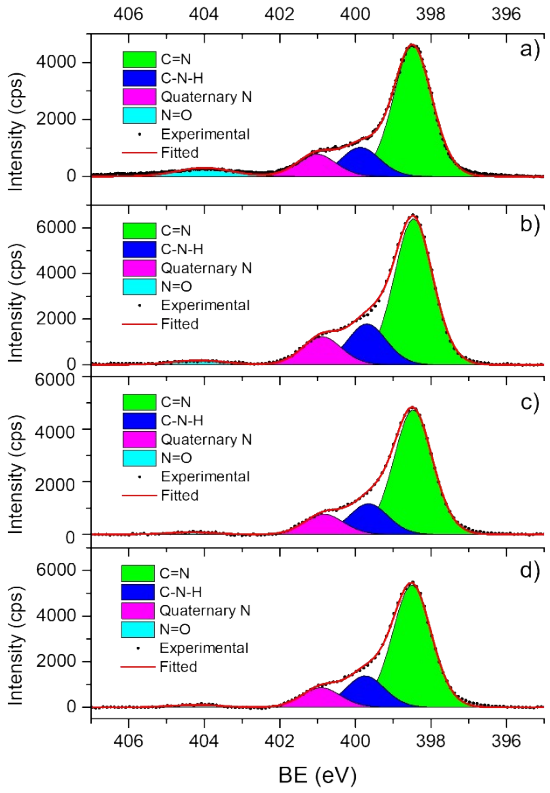

Figure S8. High resolution N 1s region for GCN samples: a) support, Ir/ GCN b) fresh, c) 1 run and d) 5 run.

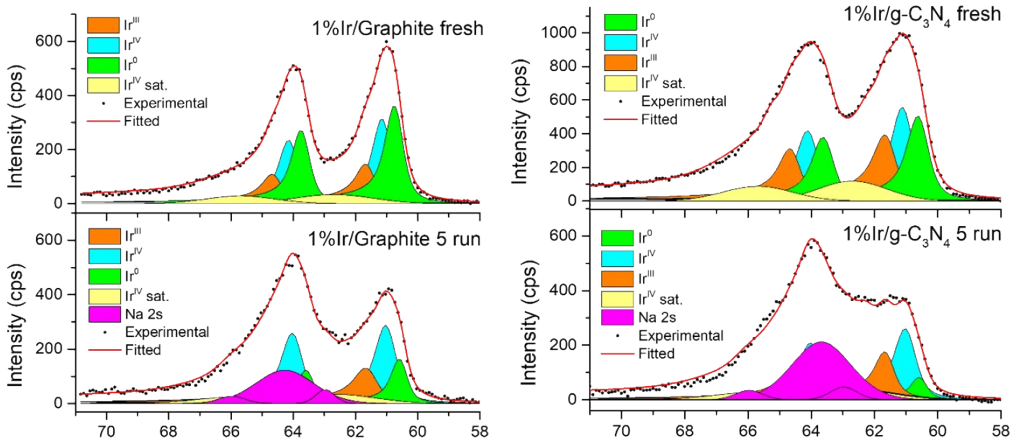

Figure S9. High resolution Ir 4f region for graphite (left panel) and GCN (right panel) samples. Na 2s interference is highlighted in magenta and overlayed to the Ir 4f region for the sake of clarity.