Electronic Supplementary Material (ESI) for RSC Advances.

Experimental and DFT studies of porous carbon covalently functionalized by polyaniline as corrosion inhibition barrier on nickel-based alloys in acidic medium.

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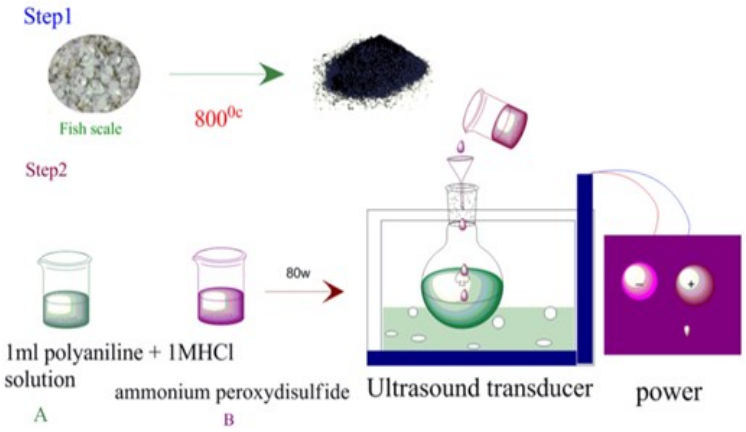


Figure S1. Scheme of the synthetic procedure of polyaniline functionalized fish-scale graphitic carbon

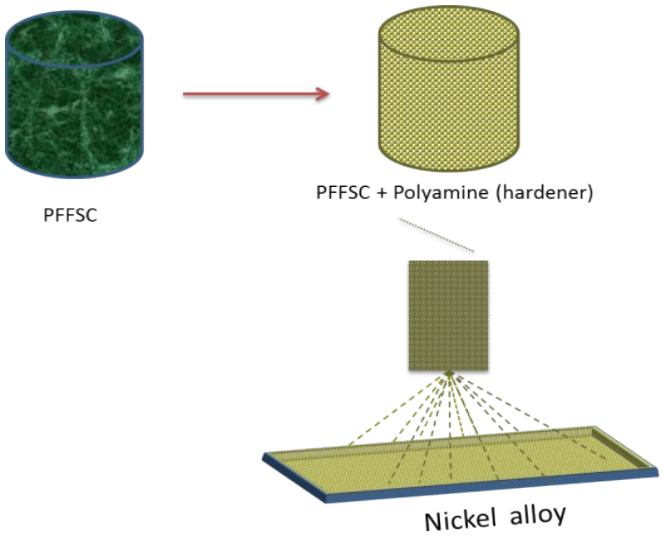


Figure S2. Schematic diagram of nickel alloy coating

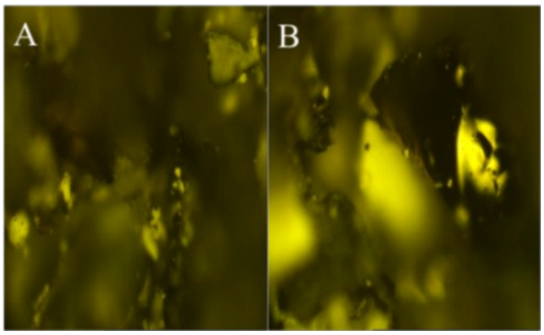
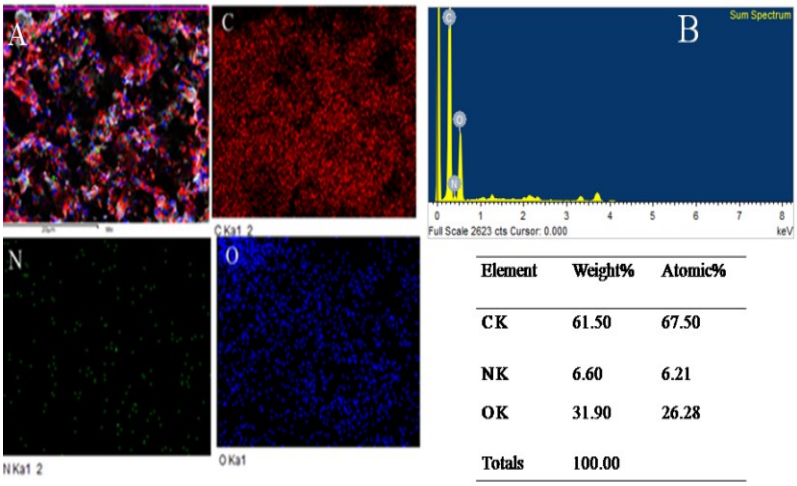


Figure S3. A) Raman image of fish-scale carbon and B) polyaniline functionalized porous carbon



Element	Weight%	Atomic%
CK	61.50	67.50
NK	6.60	6.21
OK	31.90	26.28
Totals	100.00	

Figure S4. (A) Elemental mapping of polyaniline functionalized fish-scale carbon composite materials and (B) EDX spectrum of polyaniline functionalized fish-scale carbon elements composition

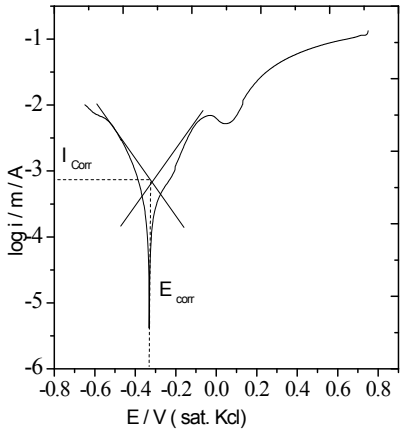


Figure S5. Schematic model of I_{corr}, and E_{corr} values calculation

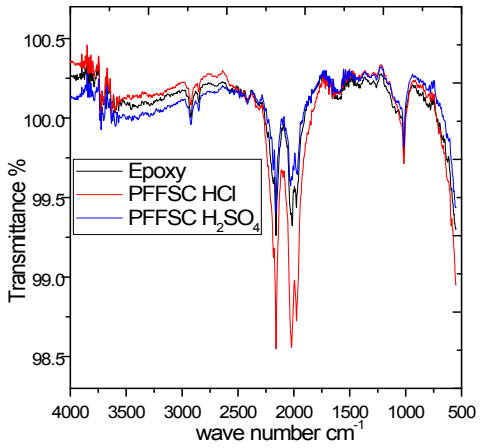


Figure S6. ATR - FTIR studies of epoxy and polyaniline functionalized fish-scale carbon coated nickel alloy immersed for 5 days in 1M HCl and 1M H_2SO_4.

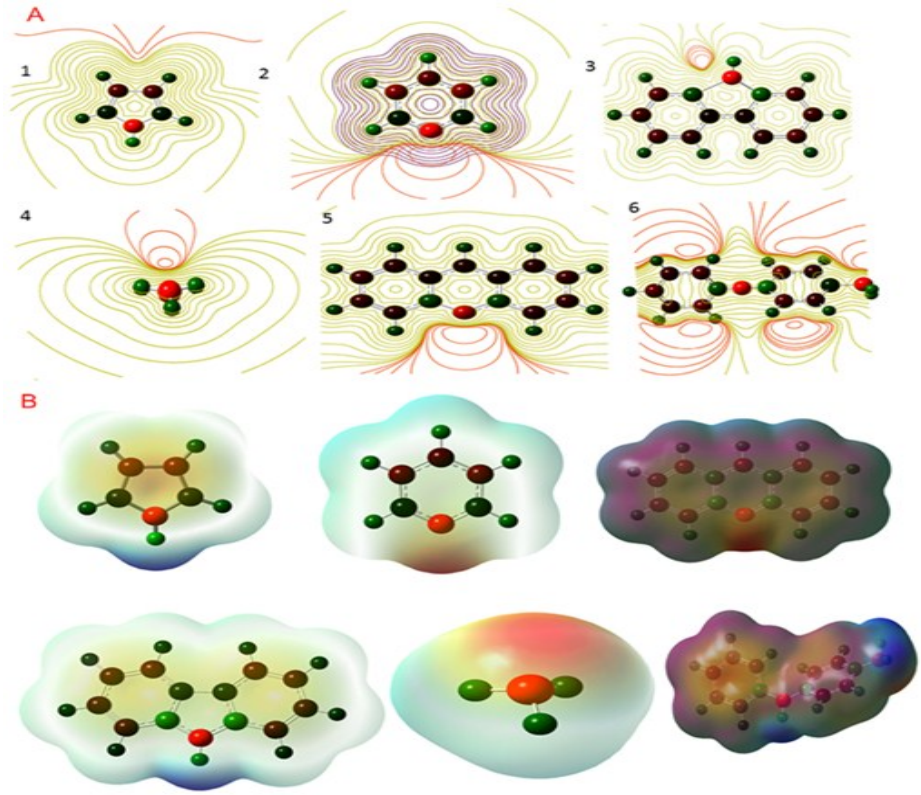


Figure S7. (A) Contour image and (B) total electrostatic potential of polyaniline fragments.

S.No	HOMO eV	LUMO eV	χ eV	η eV	σ eV	ω	ΔE_J	Dm (Debye)
GC	4.0463	3.0403	3.5433	0.5030	0.9940	12.4800	0.2575	4.7571
2GC+PANI	4.9911	1.1907	3.0909	1.9002	0.2631	3.1760	0.4705	1.4634
6GC+PANI	4.7783	1.1265	2.9524	1.8258	0.2738	1.2383	0.4564	2.2169

Table S.1 Quantum chemicals values of aniline monomer π- π interacting with fish scale graphitic carbon.