

Experimental and DFT studies of gadolinium decorated graphene oxide materials for their redox properties and as corrosion inhibition barrier layer on Mg AZ13 alloy in a 3.5% NaCl environment

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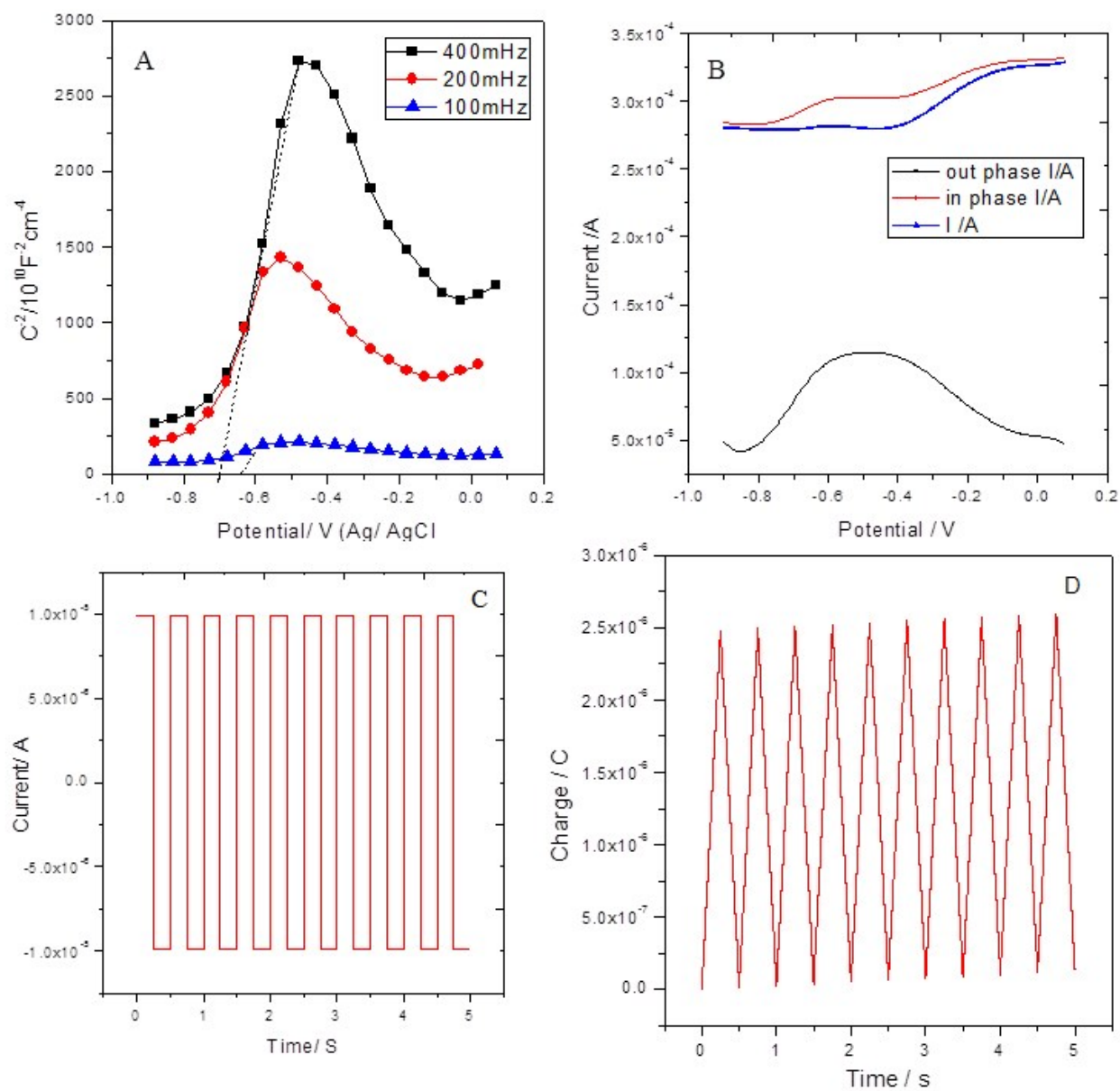


Figure S1. Motto-Schottky (a) AC-voltammetry (b) chronoamperometry (c) chronocoulometry (d) studies of Gd functionalized graphene oxide.

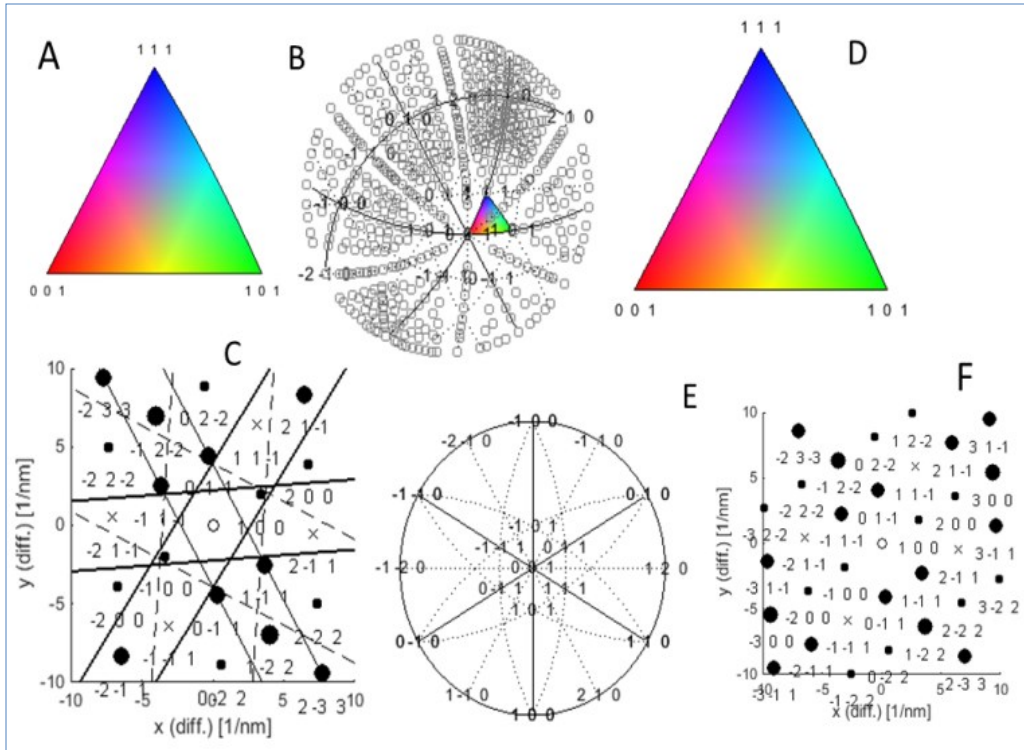


Figure S2. Epoxy and Gd+GO composite coated polycrystalline affected region of the Mg alloy surface.

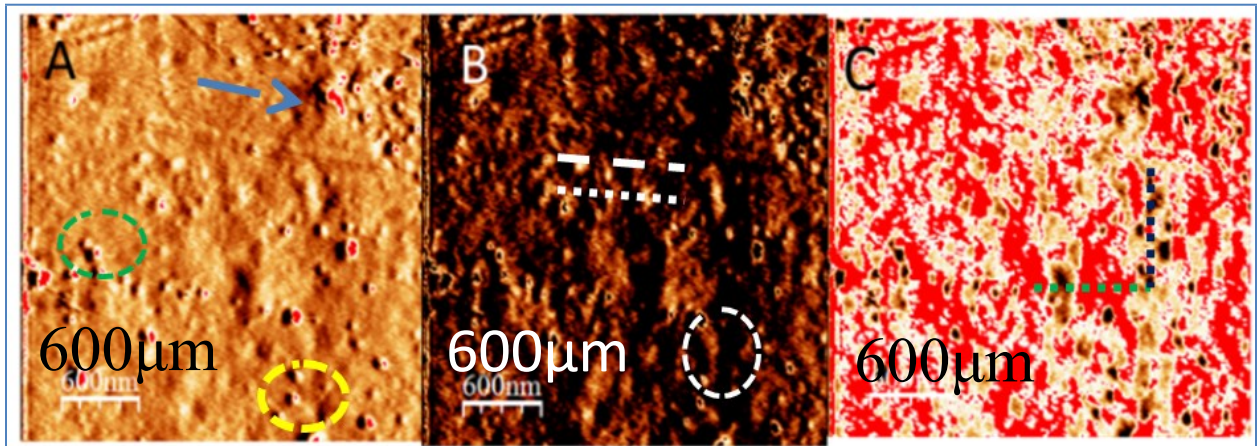


Figure S3. Topography of the epoxy coated Mg alloy immersed for 5 days in 3.5% NaCl solution.

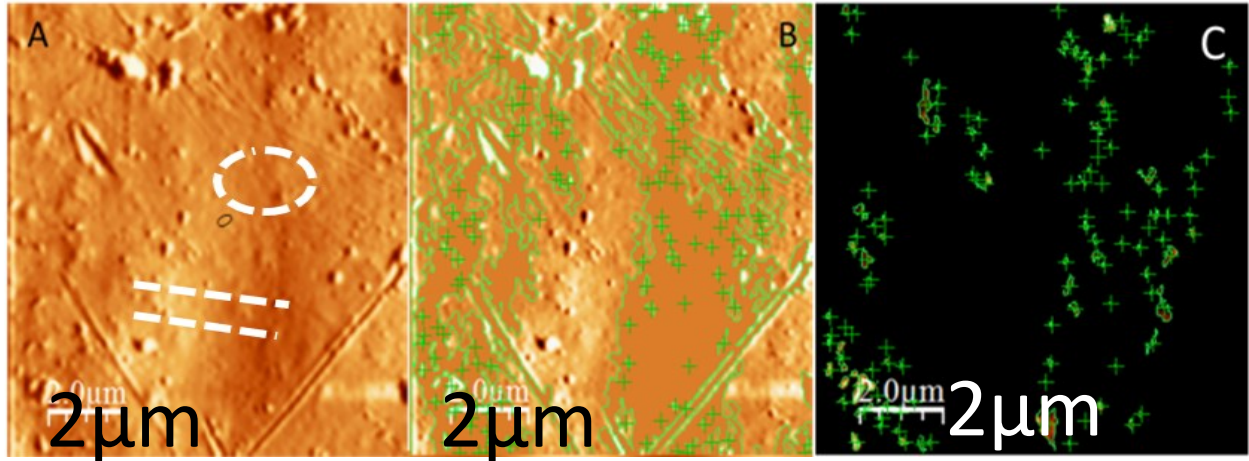


Figure S4. Topography of epoxy coated Mg alloy immersed for 5 days in 3.5% NaCl corrosion medium

S.no	$-E_{\text{Corr}}$ mV	$-I_{\text{Corr}}$ mA	LP	η	$R_{\text{Ct}}\Omega$	$C_{\text{dl}}\mu\text{F}$
Epoxy	1.385	6.42	382		450	3.5710
Gd+GO	1.899	2.61	1408	59	700	0.1136

Table S1. Epoxy and Gd+GO coated Mg alloy corrosion inhibition efficiency

	HOMO	LUMO	ΔE	I	A	χ	β	σ	ω
NEUTRAL									
A	- 0.21757	-0.16128	0.0562 9	0.2175 7	0.1612 8	0.189425	0.0281 5	35.524	0.6373 3
B	- 0.21716	-0.16033	0.0568 3	0.2171 6	0.1603 3	0.188745	0.0284 2	35.186	0.6267 5
PROTONATED									
A	- 0.22866	-0.17520	0.0534 6	0.2286 6	0.1752 0	0.20193	0.0267 3	37.411	0.7627 3
B	- 0.22859	-0.17475	0.0538 4	0.2285 9	0.1747 5	0.20167	0.0269 2	37.147	0.7554 1

Table S2. Global reactivity parameters computed for the Gd-GO system (with the implicit effects from water), for the neutral and protonated models (A.U.): HOMO-LUMO gap ΔE , ionization potential I , electron affinity A , global electrophilicity χ , global hardness η , global softness σ , and global nucleophilicity ω . A = α -HOMO & LUMO, B = α -HOMO & LUMO.