Supporting Information for the article

Facile method of synthesis of the Tb-decorated graphene oxide: electrochemical stability, hydrogen storage, and corrosion inhibition of the Mg AZ13 alloy in 3.5% NaCl medium

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Table S1. Calculated species, M062X/[Tb:SDD;C,H,O,Cl:6-31G*], gas phase/H_2O.

Spin	E_0, A.U.	E_0+ZPE, A.U.	ΔE, kcal/mol	E(HOMO/LUMO), A.U.	ΔE(HOMO/LUMO), kcal/mol/eV
C42Oxo-OTbCl3, OTbCl3 close to edge					
^{7}A	-4417.371029// -4417.445733	-4416.883078// -4416.958164	6.09	-0.24045/ -0.14410 -0.24039/ -0.14395// -0.23878/ -0.14064 -0.23872/ -0.14050	
^{5}A	-4417.351584// -4417.428218	-4416.865222// -4416.942413	17.08	-0.26441/ -0.16243 -0.22304/ -0.09470// -0.26193/ -0.15691 -0.22044/ -0.09105	
C42Oxo-O(H^+)TbCl3, OTbCl3 close to edge					
^{7}A	-4417.758153// -4417.878037	-4417.257691// -4417.378083	4.38	-0.33799/ -0.24661 -0.33796/ -0.24644// -0.24826/ -0.15258 -0.24821/ -0.15244	
C42Oxo-OTbCl3, OTbCl3 in the center					
^{7}A	-4417.378656 10i,8i// -4417.455434	-4416.889700// -4416.966634	0.0	-0.25301/ -0.14034 -0.25294/ -0.14023// -0.25043/ -0.13634 -0.25036/ -0.13623	 3.10 3.11
^{5}A	-4417.346870 9i// -4417.423066	-4416.860395// -4416.936297	20.31	-0.25996/ -0.16816 -0.21522/ -0.08637// -0.25491/ -0.16170 -0.21486/ -0.08151	
C42Oxo-O(H^+)TbCl3, OTbCl3 in the center					
^{7}A	-4417.765965// -4417.885014	-4417.264544// -4417.384042	0.0	-0.35066/ -0.24286 -0.35062/ -0.24279// -0.26057/ -0.14972 -0.26055/ -0.14968	

Table S2. M062X/[Tb:SDD; C,H,O,Cl:6-31G*], gas phase//water.

C36OH_CO2H_TbOCl3,					
^{2}A	-3886.117870//	-3885.706424//		-0.25691/ -0.13592 -0.22555/ -0.14409//	
^{6}A	-3886.332240// -3886.404255	-3885.920484// -3885.992778		-0.25690/ -0.13563 -0.22541/ -0.14382// -0.25417/ -0.12527 -0.22265/ -0.13391	
^{4}A	-3886.301625// -3886.370052	-3885.892301// -3885.960894		-0.27841/ -0.16908 -0.22136/ -0.08889// -0.27404/ -0.16284 -0.21538/ -0.08259	
OTbCl3-middle					
^{6}A	-3886.330836 9i// -3886.396833	-3885.919806// -3885.985462		-0.25417/ -0.10723 -0.21196/ -0.08931// -0.24701/ -0.09913 -0.20463/ -0.07915	