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## Correction: The corrosion inhibition of stainless steel by ferrocene–polyoxometalate hybrid molecular materials – experimental and first principles studies

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Correction for 'The corrosion inhibition of stainless steel by ferrocene–polyoxometalate hybrid molecular materials – experimental and first principles studies' by G. Sruthi *et al.*, *Phys. Chem. Chem. Phys.*, 2020, 22, 3329–3344, DOI: 10.1039/C9CP06284J.

The authors would like to make the changes described below to their published article. An updated version of the article itself with these changes incorporated is available as an additional supplementary information file alongside the original published article.

### Correction on page 3331:

The following sentence on page 3331:

"The composition of 316 grade steel is Fe: 1%; C: <0.08%; Cr: 16–18%; Ni: 10–14%; Mo: 2–3%; Mn: <2%; Si: <1%; P: <0.045%; S: <0.03%, with a molecular weight of 20.376 g mol<sup>−1</sup> and a density of 7.87 g cm<sup>−3</sup> (ASTM F138)."

Should read as:

"The composition of 316 grade steel is Fe: 60–62%; C: <0.08%; Cr: 16–18%; Ni: 10–14%; Mo: 2–3%; Mn: <2%; Si: <1%; P: <0.045%; S: <0.03%, with a molecular weight of 56.0 g mol<sup>−1</sup> and a density of 7.87 g cm<sup>−3</sup> (ASTM F138)."

Please note that accordingly the corrosion rates are also corrected. However, the corrosion inhibition efficiencies of SS@FcPW and SS@FcPMo reported remain the same.

### Corrected Figure 11(c) on page 3338:

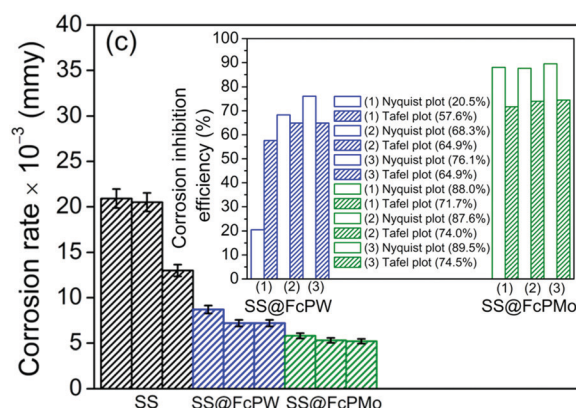


Fig. 11(c) Reproducibility tests with error bars [Fig. 11(c) is corrected, but the inset of Fig. 11(c) has no change].

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## Corrected Table on page 3339:

Table 3 Calculations from Tafel plots using Tafel extrapolation technique

Electrode	Method	$E_{\text{corr}}$ (V)	$i_{\text{corr}}$ ( $\mu\text{A cm}^{-2}$ )	Corrosion inhibition ( $\eta$ ) and corrosion rate	$\beta_a$ (V dec $^{-1}$ )	$\beta_c$ (V dec $^{-1}$ )	$R_p$ (ohm cm $^2$ )
Bare steel (SS) (316 grade)	Instr. <sup>a</sup>	−0.210	2.10	Corrosion rate = $\frac{i_{\text{corr}} \times M}{n \times F \times d}$ $= \frac{21.0 \times 10^{-7} \times 56}{2 \times 96500 \times 7.87}$ $= 7.74 \times 10^{-11} \text{ cm s}^{-1}$ $= 0.024 \text{ mmy}$	0.125	−0.068	8804
	Calc. <sup>b</sup>	−0.210	1.77	Corrosion rate = $6.52 \times 10^{-11} \text{ cm s}^{-1}$ $= 0.021 \text{ mmy}$	0.119	−0.053	8995
SS@ FcPW	Instr.	0.0100	0.62	Corrosion rate = $2.28 \times 10^{-11} \text{ cm s}^{-1}$ $= 0.0072 \text{ mmy}$ $\eta = \frac{i_{\text{corr,steel}} - i_{\text{corr,FcPW}}}{i_{\text{corr,steel}}}$ $= \frac{(17.7 - 6.2) \times 10^{-7} \times 10^2}{17.7 \times 10^{-7}} = 64.9\%$	0.102	−0.059	26 222
	Calc.	0.0100	0.62	$\eta = 64.9\%$ Corrosion rate = $2.28 \times 10^{-11} \text{ cm s}^{-1}$ $= 0.0072 \text{ mmy}$	0.108	−0.059	26 722
SS@ FcPMo	Instr.	0.0155	0.56	$\eta = 68.3\%$ Corrosion rate = $2.06 \times 10^{-11} \text{ cm s}^{-1}$ $= 0.0065 \text{ mmy}$	0.084	−0.088	33 344
	Calc.	0.0155	0.46	$\eta = 74.0\%$ Corrosion rate = $1.69 \times 10^{-11} \text{ cm s}^{-1}$ $= 0.0053 \text{ mmy}$	0.112	−0.101	37 194

<sup>a</sup> Instr. From CH Instrument software. <sup>b</sup> Calc. From Tafel extrapolation method. mmy denotes millimeter per year (mm year $^{-1}$ ).

## Correction on page 3340:

The following sentence on page 3340:

“The corrosion rates and corrosion inhibition efficiencies calculated from the Tafel extrapolation method are as follows: bare SS: 0.013 mmy; SS@FcPW: 0.009 mmy, 32%; and SS@FcPMo: 0.003 mmy, 71%.”

Should read as:

The corrosion rates and corrosion inhibition efficiencies calculated from the Tafel extrapolation method are as follows: bare SS: 0.036 mmy; SS@FcPW: 0.025 mmy, 32%; and SS@FcPMo: 0.011 mmy, 71%.

## Correction on page 3342:

The sentence on page 3342:

“From the Pearson method, we can predict the number of electrons being transferred from the inhibitor molecule to the Fe(100) surface using the expression  $[\Delta n = (\phi_{\text{Fe}} - \chi_{\text{inhibitor}})/2(\eta_{\text{Fe}} - \eta_{\text{inhibitor}})]$ , where  $\phi_{\text{Fe}}$  is the work function of Fe(110) and  $\eta_{\text{Fe}} = 0$ .<sup>74,75</sup>”

Should read as:

From the Pearson method, we can predict the number of electrons being transferred from the inhibitor molecule to the Fe(110) surface using the expression  $[\Delta n = (\phi_{\text{Fe}} - \chi_{\text{inhibitor}})/2(\eta_{\text{Fe}} - \eta_{\text{inhibitor}})]$ , where  $\phi_{\text{Fe}}$  is the work function of Fe(110) which is 4.82 eV and  $\eta_{\text{Fe}} = 0$ .<sup>74,75</sup>

## Correction in Table 4 on page 3342:

$\Delta n$  value of FcPW is 1.24 (instead of −0.22) and that of FcPMo is 1.42 (instead of −0.15).

## Correction on page 3343:

The following sentence on page 3343:

“From the table, the  $\Delta n$  values of FcPW and FcPMo are −0.22 and −0.15, respectively. These negative values indicate that both the inhibitor molecules FcPW and FcPMo act as electron acceptors from the vacant d-orbital of Fe metal on the surface of the



stainless steel plate. The electron-accepting nature of the hybrid molecules increases the adsorption of the inhibitor molecules on the metal surface, therefore inhibiting the corrosion mechanism.”

Should read as:

“From the table, the  $\Delta n$  values for FcPW and FcPMo are 1.24 and 1.42, respectively. These values indicate that the fraction of electrons is transferred from the inhibitor molecules FcPW and FcPMo to the vacant *d*-orbital of Fe metal on the surface of stainless steel plate. The fraction of electrons transferred in the case of SS@FcPMo is more than that of SS@FcPW. So, there is increased adsorption of the inhibitor molecule on the metal surface, and therefore enhanced corrosion inhibition of stainless steel in the case of SS@FcPMo.”

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

