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Correction: A unified study for water adsorption on metals: meaningful models from structural motifs

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Correction for 'A unified study for water adsorption on metals: meaningful models from structural motifs' by Guillem Revilla-López *et al.*, *Phys. Chem. Chem. Phys.*, 2014, **16**, 18933–18940.

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Authors noticed erroneous values in Table 2 that should be the result of applying the formula: $\gamma_{\text{ads}} (\text{eV } \text{\AA}^{-2}) = E_{\text{ads}}/A$ where E_{ads} are the total adsorption energies for each motif, and A the surface area where the motif was calculated.

Consequently the first paragraph of section 3.1, "Strain effects on DFT adsorption energies" from line 47 on page 18935 to line 8 on page 18936, should read:

The DFT-D2 adsorption energies for different sets of training structures under $\pm 4\%$ d_{XY} deformation are presented in Table 1 in eV per H_2O . Table 2 reports the same energies per surface area unit, $\text{\AA}^{-2}$, to better understand the experimental results. The direct comparison between data in Tables 1 and 2 indicates that the adsorption energies and surface energies follow a similar pattern. In both cases sqrt(37), 0.7 ML, shows the lowest energy. In contrast, ice-like bilayer, 0.67 ML, and Rosette, 0.5 ML, swap their position in the ranking with the latter being the least stable. Yet, in Ru(0001) dissociated ice-like bilayer has the lowest adsorption energy, γ_{ads} , followed by the other three in the same ordering.

Table 2 DFT-D2 calculated adsorption energies for H-down ice-like, sqrt(37) and Rosette structures on Pd, Pt and Ru. All energies are in $\text{eV } \text{\AA}^{-2}$. All d_{XY} are in plane deformations (in %) with respect to the unstrained metal slab

d_{XY}	Pd(111)			Pt(111)			Ru(0001)			
	Ice-like	sqrt(37)	Rosette	Ice-like	sqrt(37)	Rosette	Ice-like	Ice-like diss.	sqrt(37)	Rosette
4	−0.059	−0.071	−0.048	−0.057	−0.068	−0.047	−0.061	−0.099	−0.083	−0.059
2	−0.061	−0.072	−0.048	−0.058	−0.070	−0.047	−0.064	−0.099	−0.082	−0.059
0	−0.063	−0.073	−0.049	−0.060	−0.071	−0.047	−0.064	−0.092	−0.082	−0.058
−2	−0.064	−0.074	−0.050	−0.061	−0.072	−0.047	−0.064	−0.084	−0.083	−0.057
−4	−0.065	−0.075	−0.049	−0.063	−0.073	−0.047	−0.066	−0.075	−0.083	−0.056

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