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## CORRECTION



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

Guillem Revilla-López\* and Núria López\*

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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:  $\gamma_{ads} (eV \AA^{-2}) = E_{ads}/A$  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<sub>2</sub>O. Table 2 reports the same energies per surface area unit, Å<sup>-2</sup>, 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,  $\gamma_{ads}$ , 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 eV Å<sup>-2</sup>. All  $d_{XY}$  are in plane deformations (in %) with respect to the unstrained metal slab

|          | Pd(111)  |          |         | Pt(111)  |          |         | Ru(0001) |                |          |         |
|----------|----------|----------|---------|----------|----------|---------|----------|----------------|----------|---------|
| $d_{XY}$ | 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.

Institute of Chemical Research of Catalonia, ICIQ, Av. Països Catalans 16, 43007 Tarragona, Spain. E-mail: nlopez@iciq.es