Corrigendum

Title: Corrigendum to Catalytic dissociation of a water molecule on the (111) surfaces of $Pt_{0.5}Ni_{0.5}$ bimetal: Density functional theory (DFT) study

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The authors regret Equation 5 in the paper has an error, not showing all sublayers for each surface explored and omitting comparison of surface energy data with other publications.
The authors would like to apologise for any inconvenience caused.

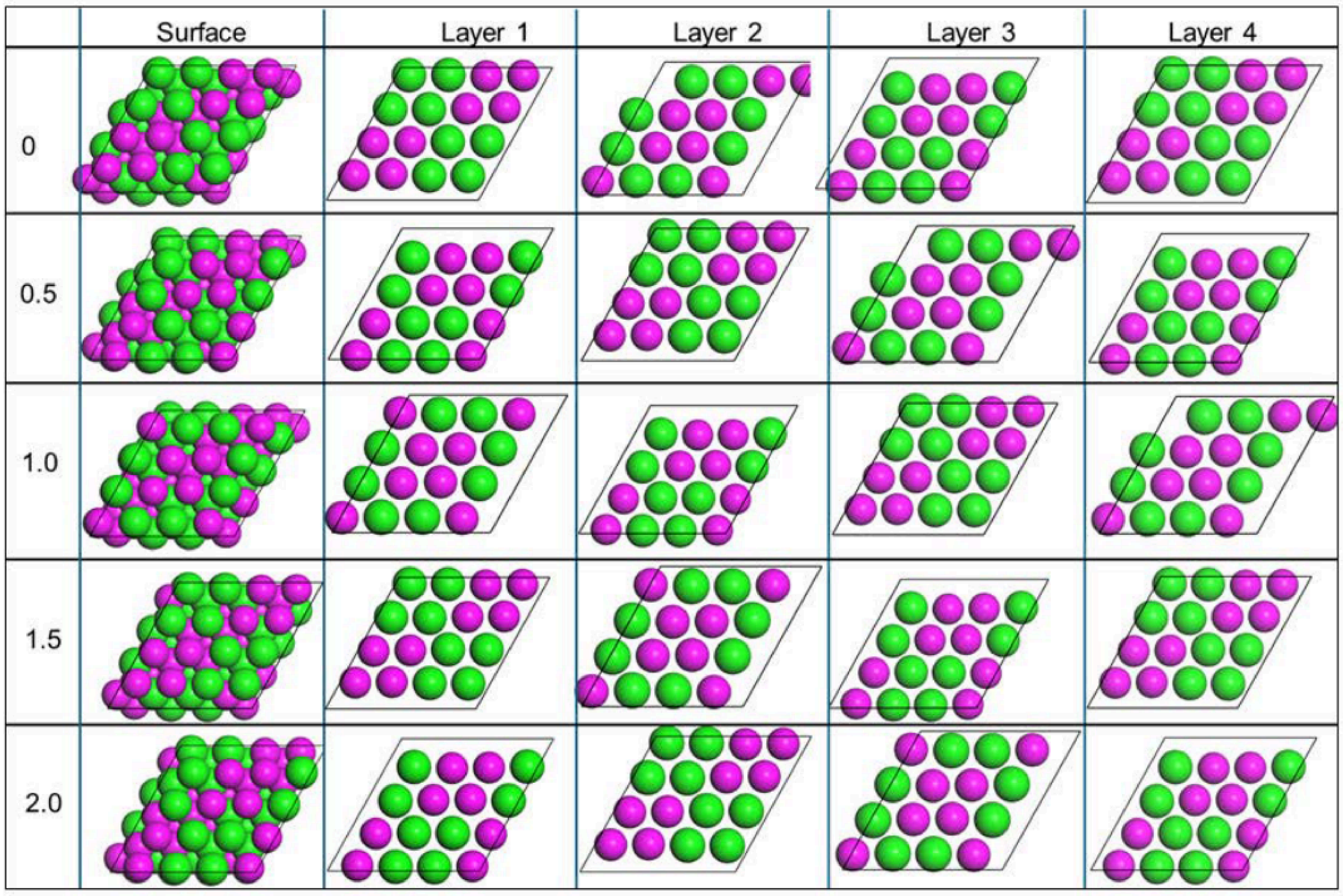
1) Correction in the formula for the surface energy

For the unrelaxed surface energy, it is always compared to the relaxed bulk structure. Even though there is a typo in the given formula, the correct values were used to obtain γ_u given in Table 1.

$$\gamma u = \left[\frac{E_{\text{slab}}^{\text{unrelaxed}} - nE_{\text{bulk}}^{\text{relaxed}}}{2A} \right] \quad \textbf{(5)}$$

2) Explanation on the various surface cuts

Figure 2 in the paper shows a schematic representation of the Pt0.5Ni0.5 bulk cleaving process by changing the fractional cleave depth (Pt in green, Ni in pink). It was not made clear how the sublayers of each slab model changed.



Various terminations of the $Pt_{0.5}Ni_{0.5}$ (111) are the same, however, sublayers are shifted. The nearest neighbours of atoms within these surfaces directly influence their properties. [1-4] Therefore, it was reasonable to examine all surface terminations, even those that appear similar, to determine whether deeper layers could affect the surface characteristics.

Across the different (111) surface terminations (0.0, 0.5, 1.0, 1.5, and 2.0), the Ni–Ni and Pt–Pt distances remained largely constant, with Δ_{relax} values of – 0.08 Å for Ni–Ni and 0.03 – 0.04 Å for Pt–Pt, corresponding to minor percent changes (1.8 – 2.1%). The Pt–Ni bond exhibited slightly higher deviations in Δ_{relax} (– 0.04 to – 0.03 Å) and percent changes (1.6 – 6.3%). Overall, these results indicate that the bimetallic surfaces are structurally identical, maintaining stability across all surface terminations, with only minimal atomic movement required during relaxation. This stability and structural similarity also result in compatible surface energies, as reported in Table 1 of the published paper. Only 3 terminations (0, 0.5, 1.0) have different sublayers, after which that is repeated.

3) Comparison of the surface energies for the pure Pt and Ni (111) surfaces compared to other works by same authors

A subset of the authors has previously conducted a related study using VASP with PBE, GGA, and plane-wave functionals to investigate H_2O adsorption on Pt surfaces [5]. However, a direct comparison with the present work—performed using CASTEP with PBE, GGA, and a localized basis set—was not included.

In the 2019 paper [5], the authors stressed that the pure DFT results underestimated the surface energies (0.866 J/m^2), overestimated with DFT-D2 (3.961 J/m^2) and gave the best results with DFT-D3(BJ) (2.046 J/m^2) when compared to the experimental value of 1.49 J/m^2 [6]. In this work, even though a very different simulation method was used, the surface energy (1.3429 J/m^2) correlated very well with said experimental values. Indeed, we would like to clarify that the use of ultra soft pseudopotential in this work as opposed to projector augmented-wave functions in the previous work means that the methods are not directly comparable and an energy difference of ~40% is well within the expected range [7].

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