Erratum: "On the tautomerisation of porphycene on copper (111): Finding the subtle balance between van der Waals interactions and hybridisation" [J. Chem. Phys. 145, 244701 (2016)]

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We have found an error in the calculations involving the functional vdW-DF-cx reported in Table II and Fig. 4 of Ref. 1. The corrected results are shown here in Table I and Fig. 1. With the corrected values, vdW-DF-cx belongs to the category of functionals that are too attractive for this system, such as optB88-vdW or vdW^{surf}. This does not alter the conclusions of the paper, where we find that vdW-DF(PBE) provides the optimal balance of short and long-range interactions.

TABLE I. Adsorption energy difference between *cis* and *trans* configurations on Cu(111), and molecule heights measured as the average height $\tilde{z}$ of the centres of mass of the four pyrroles in each molecule for the vdW-DF-cx functional.

Functional	E_{c-t} (eV)	$\tilde{z}_{trans}$ (Å)	$\tilde{z}_{cis}$ (Å)
vdW-DF-cx	−0.086	2.42	2.54

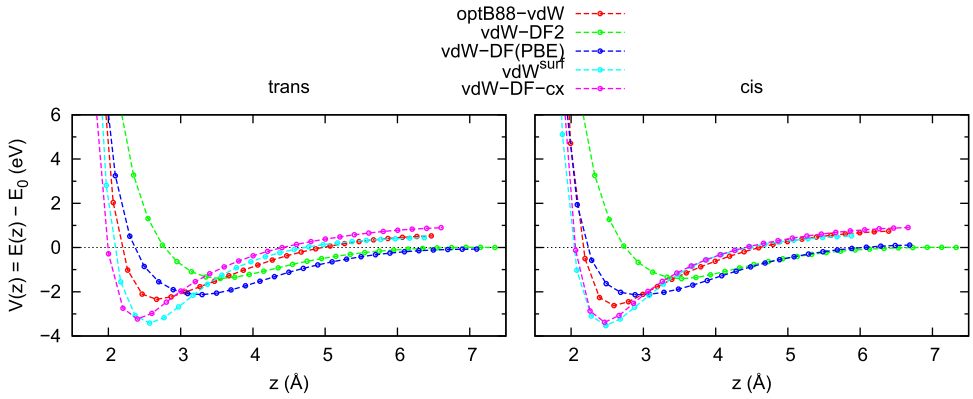

FIG. 1. Adsorption potential (one-dimensional PES) for porphycene approaching the Cu(111) surface. The z values represent the molecule height (measured as the average height of the N atoms) for equispaced rigid shifts of the unrelaxed molecule. The energy zero of each potential curve indicates the adsorption energy E_0 with respect to the relaxed gas-phase molecular geometry.

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