

Erratum: Influence of van der Waals forces on the adsorption structure of benzene on silicon studied using density functional theory [Phys. Rev. B 77, 121404 (2008)]

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The PBE energies in Table I of the original paper should be 1.16 eV and 0.89 eV for the tight-bridge (TB) and butterfly (BF) structures, respectively. In Tables II and III the reported PBE energies were, in fact, PW91 energies and the revPBE energies were incorrect. The corrected versions of Tables II and III are below and for clarity we have included both the PW91 and PBE energies. The conclusions of the original paper are not affected.

TABLE II. vdW-DF E_{ads} and its contributions, are shown for a coverage of 0.5 ML. The standard DFT PW91, PBE and revPBE results are shown for comparison. All energies are in eV.

	PW91	PBE	revPBE	vdW-DF	E^{vdWO}	E_{nl}^{c}
BLS (BF)	3.51	3.45	3.03	3.32	1.96	1.36
BLS (TB)	8.51	8.45	7.98	8.02	6.56	1.46
IMM (BF)	0.00	-0.03	-0.05	0.02	-0.04	0.06
IMM (TB)	-0.03	-0.06	-0.07	-0.02	-0.07	0.05
UF (BF)	-2.52	-2.52	-2.51	(-2.52)		
UF (TB)	-7.23	-7.23	-7.24	(-7.23)		
E_{ads} (BF)	0.99	0.89	0.47	0.82		
E_{ads} (TB)	1.24	1.16	0.66	0.77		

TABLE III. Variation of adsorption energy with coverage for the BF and TB structures. The PW91, PBE and revPBE results are also shown for comparison. All energies are in eV.

	PW91	PBE	revPBE	vdW-DF
BF-0.5	0.99	0.89	0.47	0.82
BF-0.25a	1.02	0.93	0.51	0.82
BF-0.25b	1.02	0.93	0.61	0.84
BF-0.125	1.04	0.96	0.54	0.84
TB-0.5	1.24	1.16	0.66	0.77
TB-0.25a	1.23	1.16	0.67	0.74
TB-0.25b	1.33	1.25	0.76	0.86
TB-0.125	1.31	1.24	0.75	0.82