Erratum: Adsorption and bonding mechanism of a N,N′-di(*n*-butyl)quinacridone monolayer studied by density functional theory including semiempirical dispersion corrections [Phys. Rev. B 78, 165432 (2008)]

J.-H. Franke, V. Caciuc, L. F. Chi,* and H. Fuchs

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Unfortunately, the C_6 coefficients of the dispersion corrections we used were different from the original scheme of Grimme. We changed this and found that the most important change with respect to the data presented in the paper are the underestimation of the interactions with the substrate. However, the conclusions drawn in the paper concerning the dispersion corrections remain valid when using the original coefficients of Grimme. Using these, we obtain the following values for the binding energy and bond lengths (Tables I and II in the paper):

The net effect is a stronger binding to the substrate, bringing the DBQA molecule closer to the substrate by 1.2 Å for configurations **1** and **2** and 0.5 Å for configurations **3** and **4** when compared to the PBE calculations. In the paper these values are 0.7–0.8 Å and 0.25 Å. Also for configurations **1** and **2** we find Ag-O bonds. Correspondingly, the binding energies are also higher for all configurations as given in the table, but the general site-unspecific character of the dispersion forces leads to the same energy ordering (with the exception of exchanged configurations **1** and **2**).

The difference between the electronic structure to the paper is small with only minimal changes to the work function change and the PDOS. This is exemplified by Figs. 1 and 2. Figure 1 contains the local potential plot for the dispersion forces (Fig. 6 in our paper) and Fig. 2 the PDOS of configurations **2** and **4** (bottom row of Fig. 7 in our paper).

TABLE I. Table I of the paper with the original C_6-coefficients.

	Binding Energy		Dipole moment (eÅ)		Work function change (eV)	
Configuration	PBE	PBE+D	PBE	PBE+D	PBE	PBE+D
DBQA monolayer, Arm down	−0.181	−0.447	0.0	0.0		
DBQA monolayer, Arm up	−0.133	−0.462	−0.255	−0.371		
Arm down, oxygen on hollow site **(1)**	−0.229	−3.839	−0.769	−1.213	−0.48	−0.76
Arm up, oxygen on hollow site **(2)**	−0.316	−3.809	−0.668	−1.088	−0.42	−0.68
Arm down, oxygen on top site **(3)**	−0.377	−4.261	−1.362	−1.142	−0.85	−0.71
Arm up, oxygen on top site **(4)**	−0.492	−4.282	−1.308	−1.094	−0.81	−0.68

TABLE II. Table II of the paper with the original C_6-coefficients.

	Bond lengths (Å)							
	DFT-PBE				DFT-PBE+D			
Bond	(1)	(2)	(3)	(4)	(1)	(2)	(3)	(4)
Ag-O1	4.18	4.47	2.44	2.48	2.49	2.41	2.28	2.30
Ag-O2	4.11	4.11	2.46	2.44	2.35	2.78	2.30	2.29
Ag-O3	4.35	4.61	2.45	2.48	2.43	2.41	2.28	2.30
Ag-O4	4.33	4.46	2.46	2.44	2.38	2.78	2.30	2.29
C1-Sub	4.04	4.06	3.30	3.10	2.90	2.86	2.68	2.58
C2-Sub	3.98	3.91	3.11	3.10	2.70	2.70	2.59	2.56
C3-O1	1.276	1.277	1.296	1.298	1.303	1.305	1.311	1.314
C4-O2	1.277	1.276	1.299	1.298	1.308	1.295	1.315	1.312

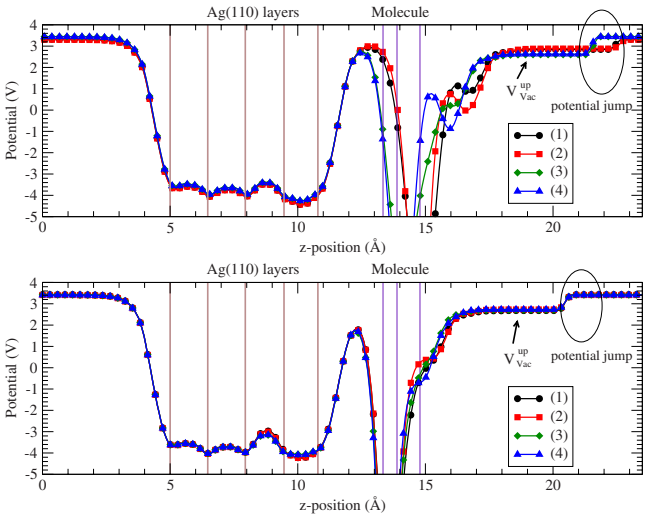

FIG. 1. (Color online) Figure 6 of our paper (dispersion part only) with the original C_6-coefficients.

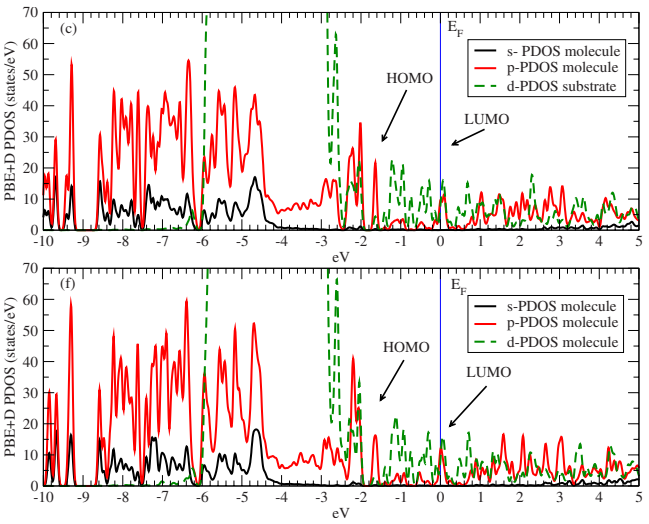

FIG. 2. (Color online) Bottom row of Fig. 7 of our paper with the original C_6-coefficients.

*chi@uni-muenster.de