

Strathprints Institutional Repository

Johnston, Karen and Kleis, Jesper and Ludqvist, Bengt I. and Nieminen, Risto M. (2008) *Erratum: Influence of van der Waals forces on the adsorption structure of benzene on silicon studied using density functional theory (vol 77, art no 121404, 2008).* Physical Review B: Condensed Matter and Materials Physics, 77 (20). ISSN 1098-0121

Strathprints is designed to allow users to access the research output of the University of Strathclyde. Copyright © and Moral Rights for the papers on this site are retained by the individual authors and/or other copyright owners. You may not engage in further distribution of the material for any profitmaking activities or any commercial gain. You may freely distribute both the url (http:// strathprints.strath.ac.uk/) and the content of this paper for research or study, educational, or not-for-profit purposes without prior permission or charge.

Any correspondence concerning this service should be sent to Strathprints administrator: mailto:strathprints@strath.ac.uk

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)]

Karen Johnston, Jesper Kleis, Bengt I. Lundqvist, and Risto M. Nieminen (Received 30 April 2008; published 30 May 2008)

DOI: 10.1103/PhysRevB.77.209904 PACS number(s): 68.43.Bc, 31.15.es, 34.35.+a, 71.15.Mb, 99.10.Cd

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	$E^{ m vdWO}$	$E_{\rm nl}^{\rm c}$
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)		
$E_{\rm ads}({\rm BF})$	0.99	0.89	0.47	0.82		
$E_{\rm ads}$ (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 V.

	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