Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Tuning the work function of the silicene-4x4 Ag(111) surface

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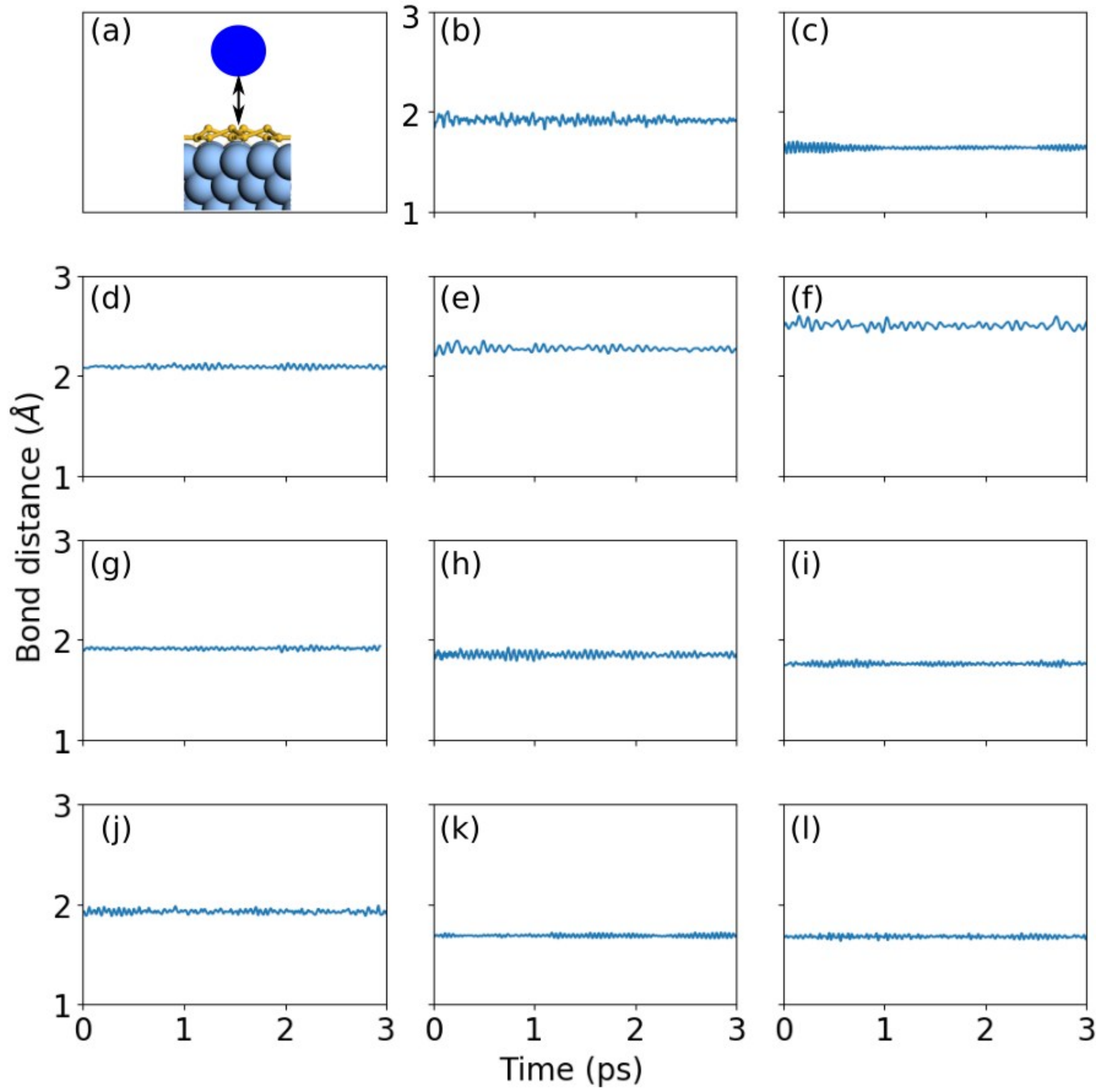

Figure S1: The bond distance between the Si atom and the covalently bonded atom in the respective functional group. A schematic of the structure is displayed in (a). The calculated variation in bond distances are for (b) the surface functionalised with (b) six phenyl (C_6H_5) groups, (c) six fluorine (F) atoms, (d) six chlorine (Cl) atoms , (e) six bromine (Br) atoms, (f) six iodine (I) atoms, (g) six methyl (CH_3) groups, (h) six cyano (CN) groups, (i) six amino (NH_2) groups, (j) six ethylmethylamine ($(CH_{2})_2NHCH_3$) groups, (k) six hydroxyl (OH) groups and (l) six methoxy (OCH_3) groups.

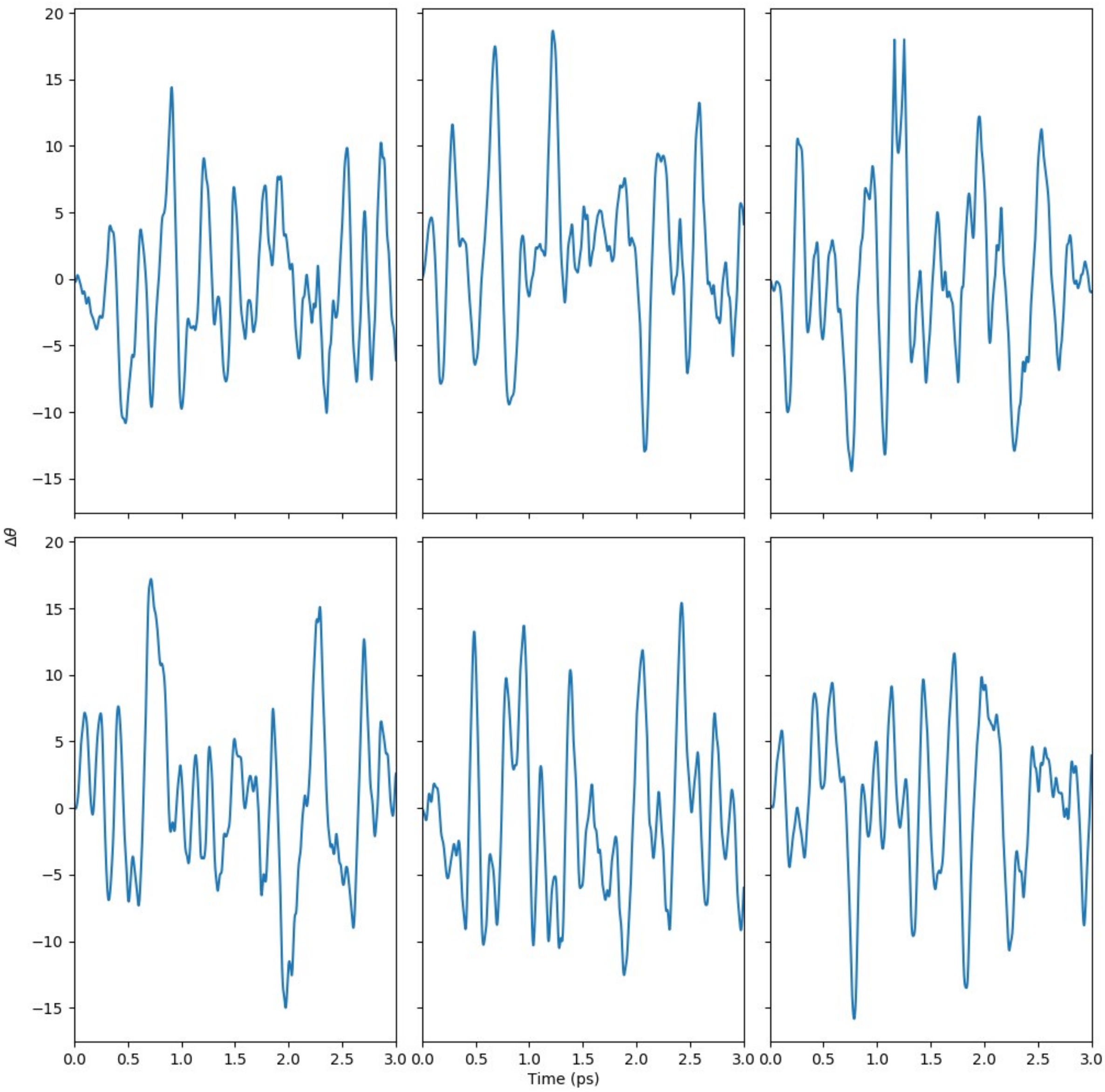

Figure S2: The variation in the horizontal orientation, in degrees, for each of the 6 phenyl groups in the structure in Fig. 2(b) as a function of time. The unit of the variation in the angles, $\Delta\theta$, is in degrees.

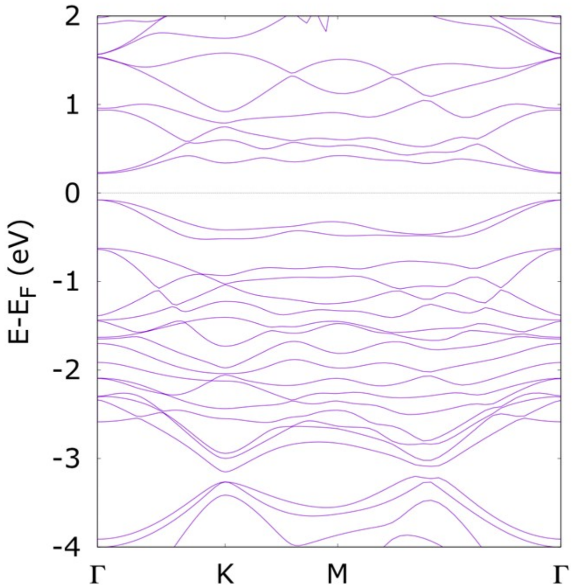

Figure S3: The electronic band structure for the free-standing silicene monolayer, with the Si atoms frozen to coordinates position.

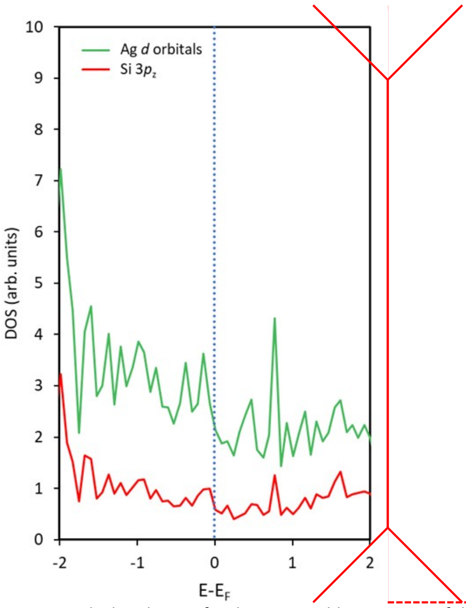

Figure S4: Calculated PDOS for the most stable geometry of the pristine Si/Ag(111) showing a zoomed in region around the fermi level.

Comment [SA]: Label: Ag 4d