S1 Supplementary Information for:

Phthalocyanine reactivity and interaction on the 6H-SiC(0001)-(3×3) surface by core-level experiments and simulations

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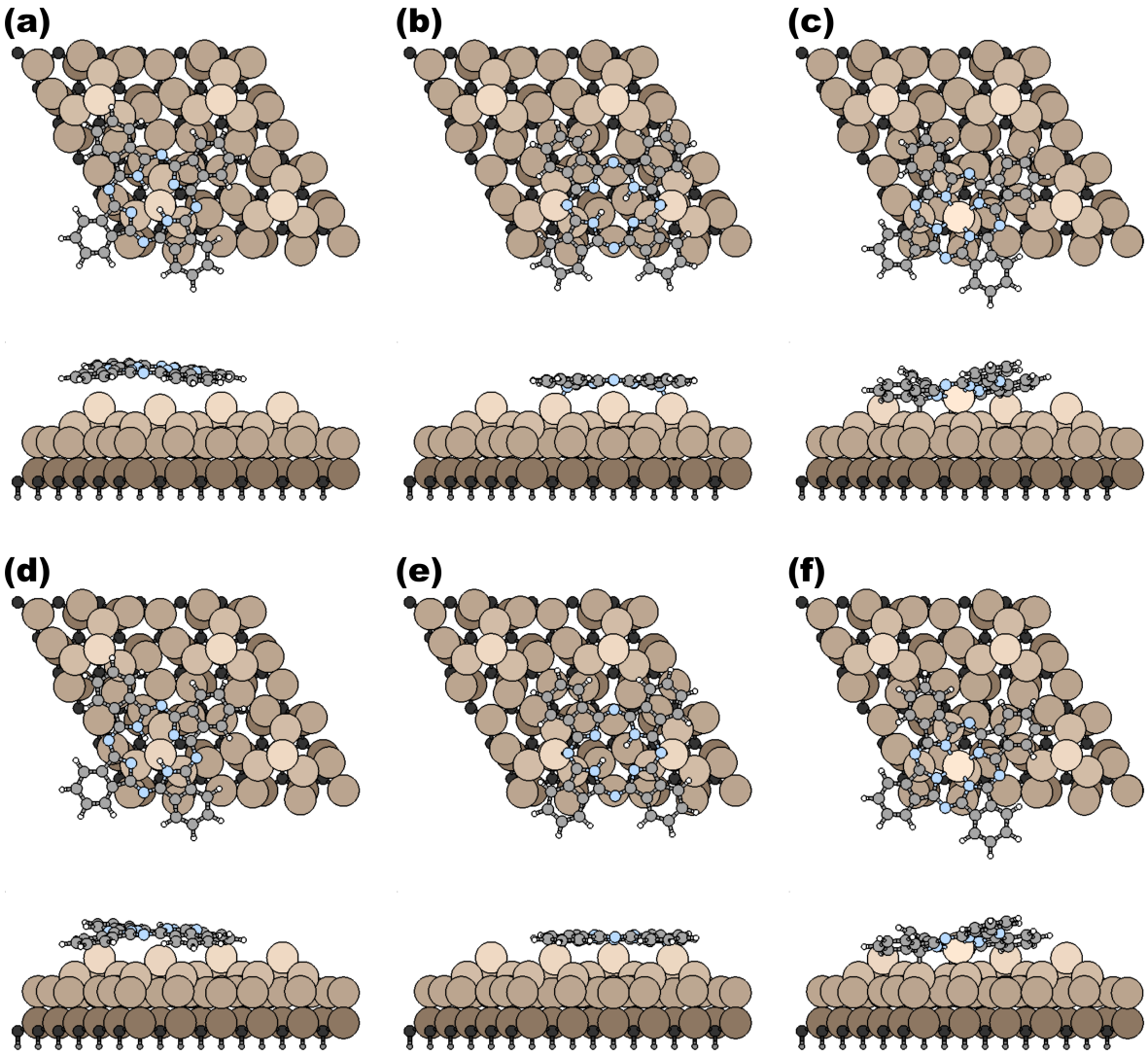

Fig. S1 Comparison between optimized structures with GGA-PBE (as presented in the main text, panels a-c) and with dispersion forces at the PBE+D2 level (panels d-f) for (a,d) top and (b,e) bridge positions of H_2Pc/6H-SiC(0001)-(3×3), (c,f) top positioned SiPc/6H-SiC(0001)-(3×3). Top/bottom panels show top/side views, respectively. The coloring is as follows: C-gray, N-blue, H-white, Si-brown, with over imposed darkening according to atom height.

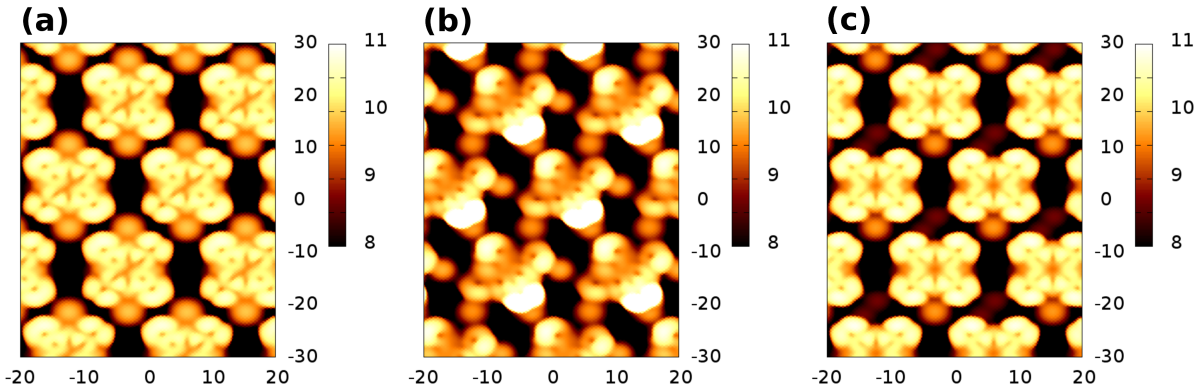

Fig. S2 Comparison of the simulated STM images for H_2Pc/6H-SiC(0001)-(3×3) adsorption configurations: (a) H_2Pc in the bridge site, (b) SiPc top, (c) SiPc bridge. Heights reported as a color scale are evaluated following an isolevel of the electronic local density of states integrated in the valence band until -2 eV. All values in Å.

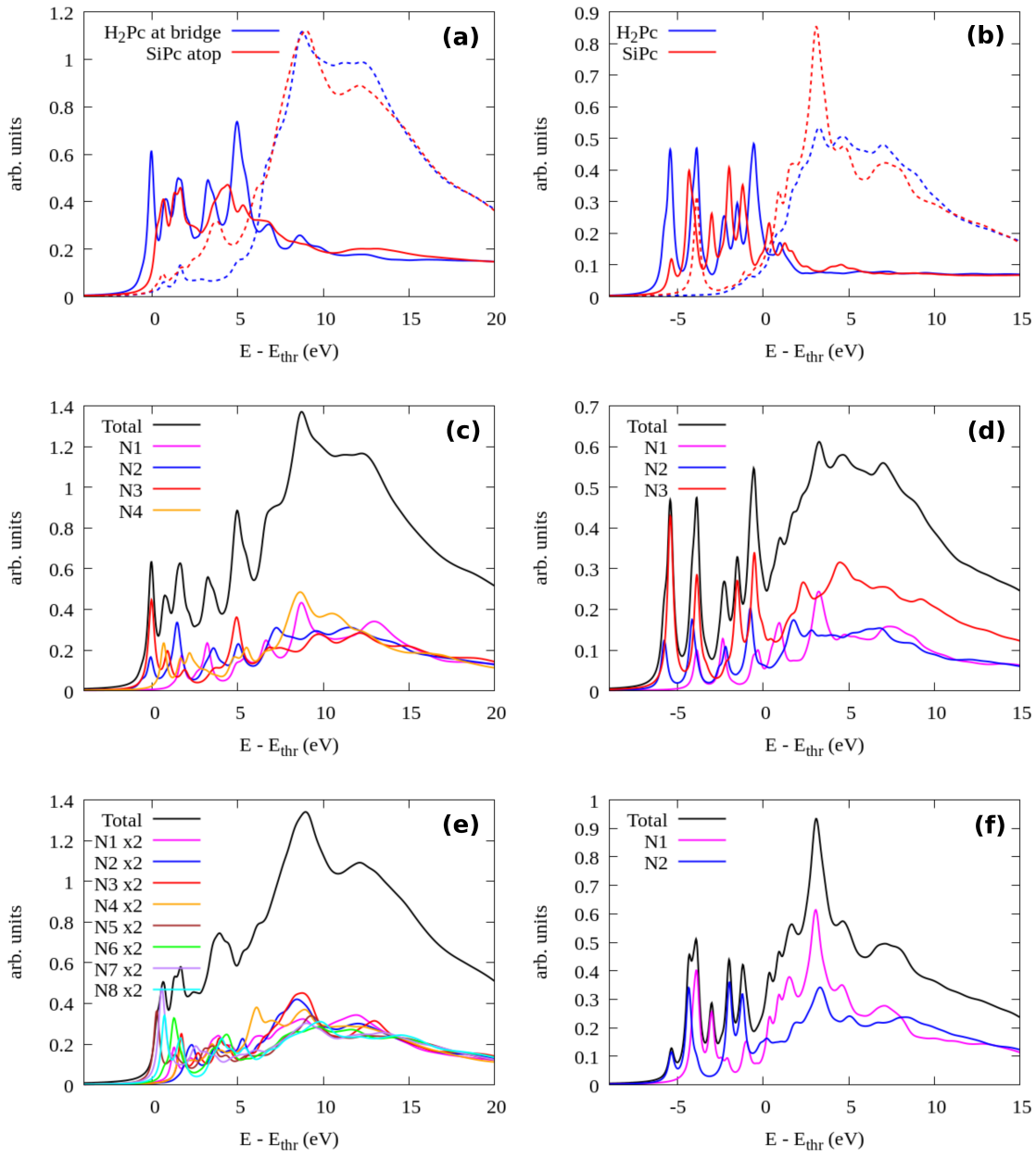

Fig. S3 Comparison of the simulated N 1s NEXAFS between (a) bridge H_2Pc/6H-SiC(0001)-(3×3) and top SiPc/6H-SiC(0001)-(3×3), (b) Gas phase H_2Pc and SiPc. The solid lines represent photon polarization along the surface normal and the dotted ones in the surface plane. The contributions from all the inequivalent atoms to the total spectrum are shown next for (c) H_2Pc/6H-SiC(0001)-(3×3), (d) gas phase H_2Pc, (e) SiPc/6H-SiC(0001)-(3×3), and (f) gas phase SiPc.