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Electronic Supplementary Information:

Self-ordering of chemisorbed PTCDA molecules on Ge(100) driven by repulsive forces

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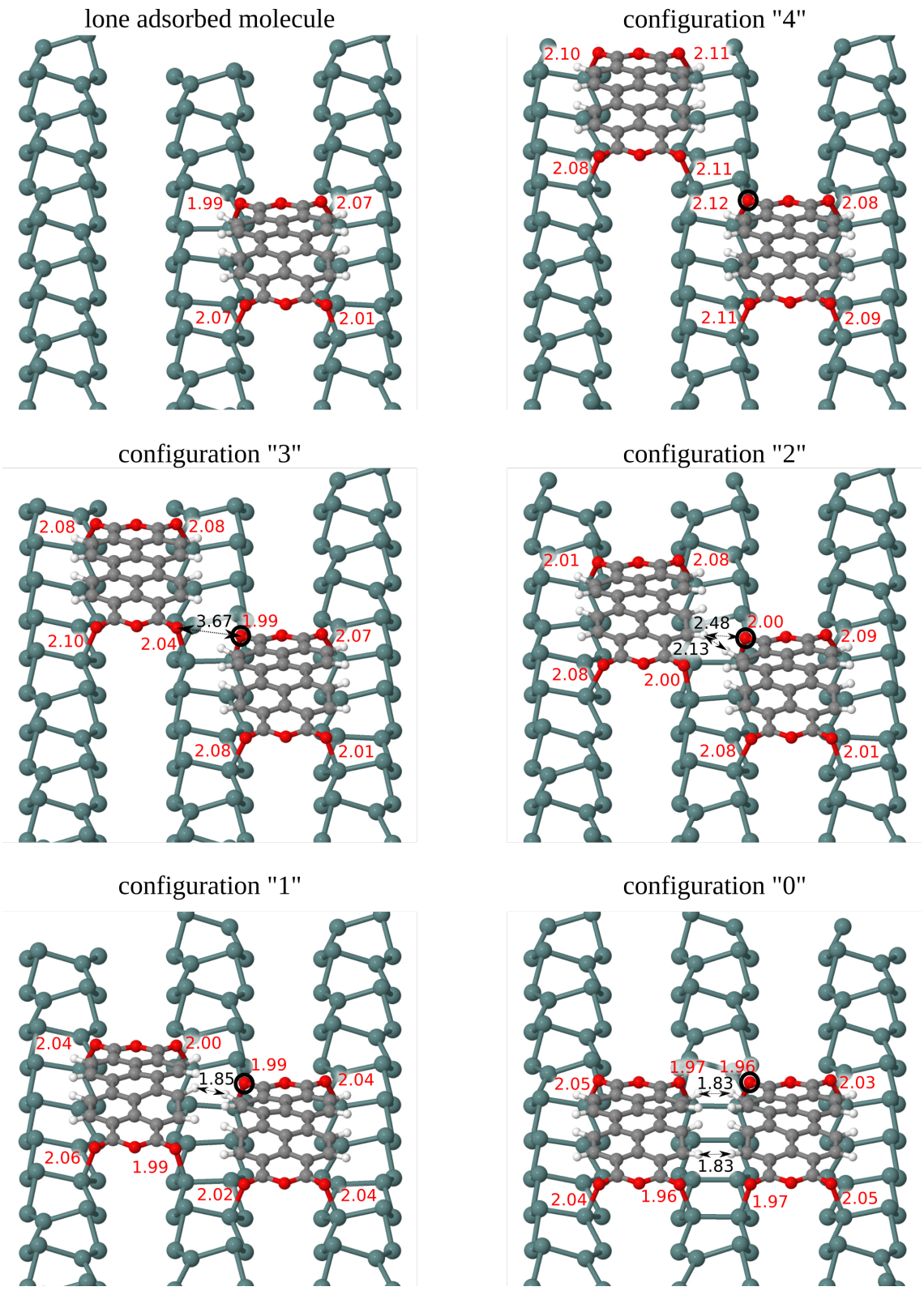

Fig. S1 Top-side views of DFT-relaxed structures of various configurations. Only molecules and two topmost Ge layers are shown. Red labels indicate lengths of Ge-O bonds, black labels indicate distances between selected atoms. All values are in Å.

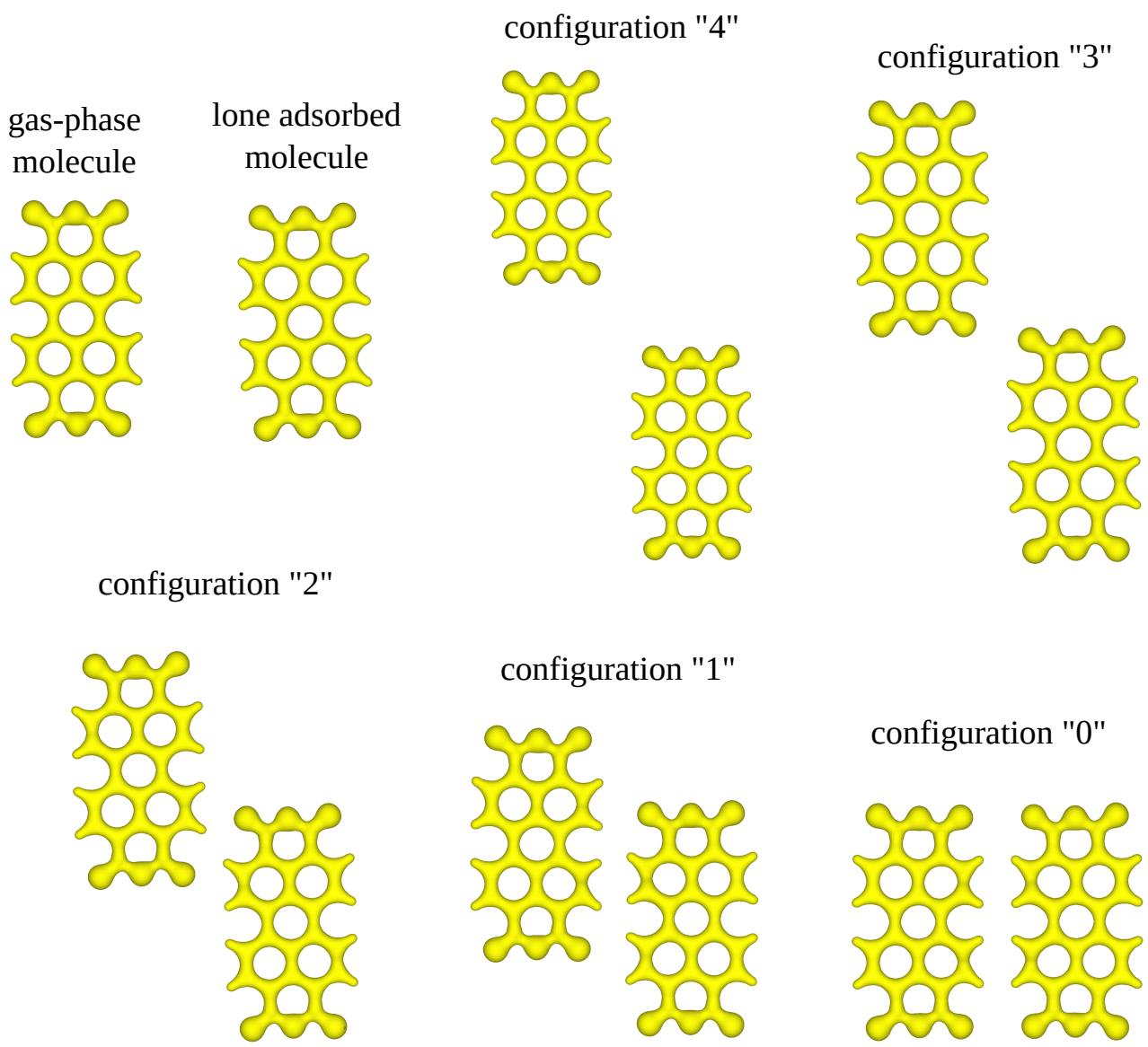

Fig. S2 Isosurfaces of the total charge distributions of PTCDA molecules at different configurations as calculated by DFT. Only the densities related to the molecules are visualized. Comparison shows that the charge distribution does not change significantly upon adsorption on the Ge(001) surface nor by presence of a nearby molecule.

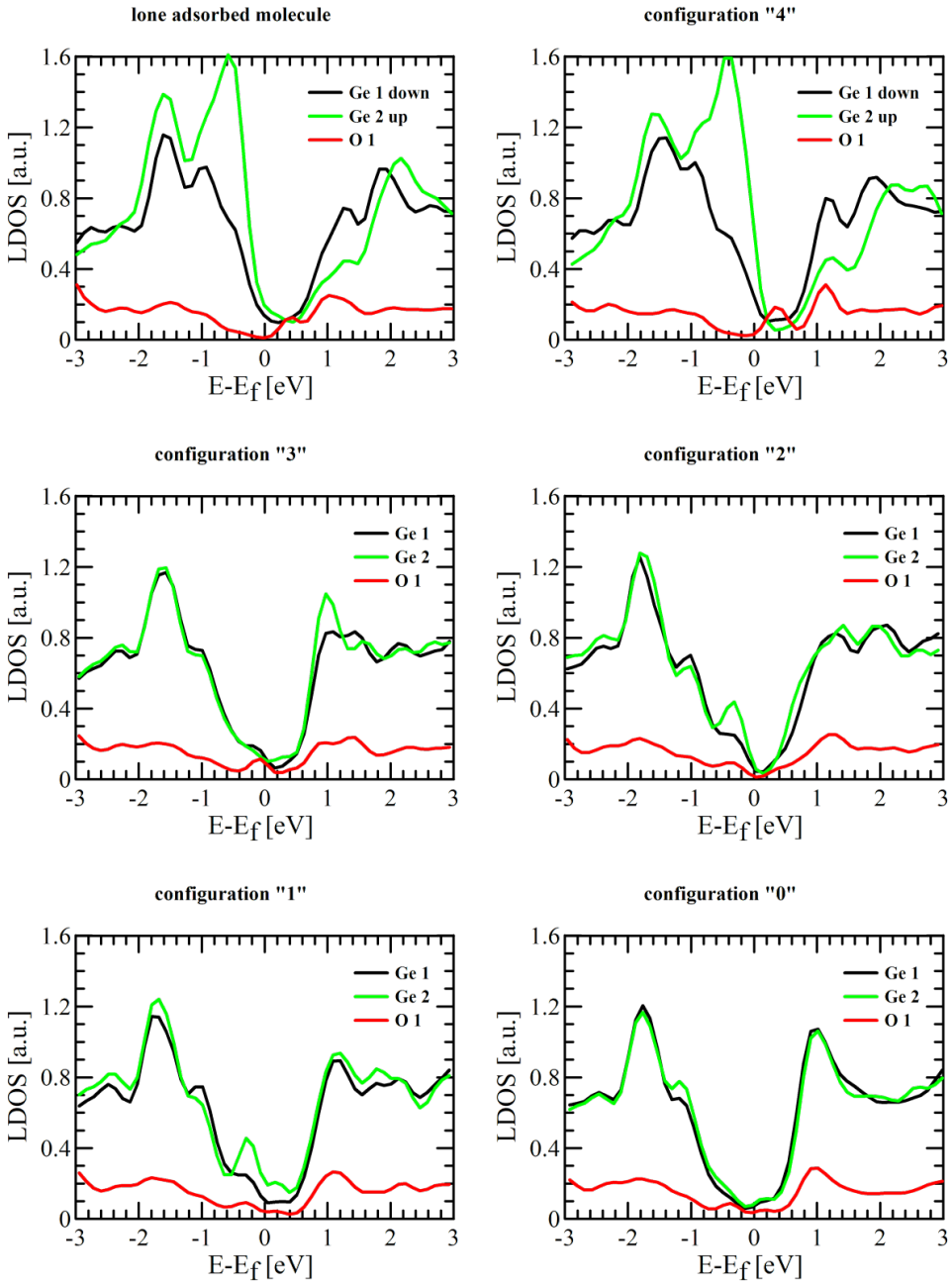

Fig. S3 Local densities of states projected onto the orbitals of selected atoms: O1 are the carbonyl oxygen atoms marked by circles in the corresponding models in Figure **??**, while Ge1 and Ge2 form the Ge dimer, to which (via Ge1) the O1 atom is bonded. The densities indicate that in configuraions "0", "1", "2" and "3" there is an indirect interaction between both molecules via germanium dimers which are in contact with these molecules. As a result, these dimers become almost completly flat which modifies also LDOS distributions associated with O atoms interacting with these dimers. Such situation does not take place in configuration "4" which let us to treat molecules in this configuration as quasi-isolated.