

Supporting Information for

Interaction of a conjugated polyaromatic molecule with a single dangling bond quantum dot on a hydrogenated semiconductor

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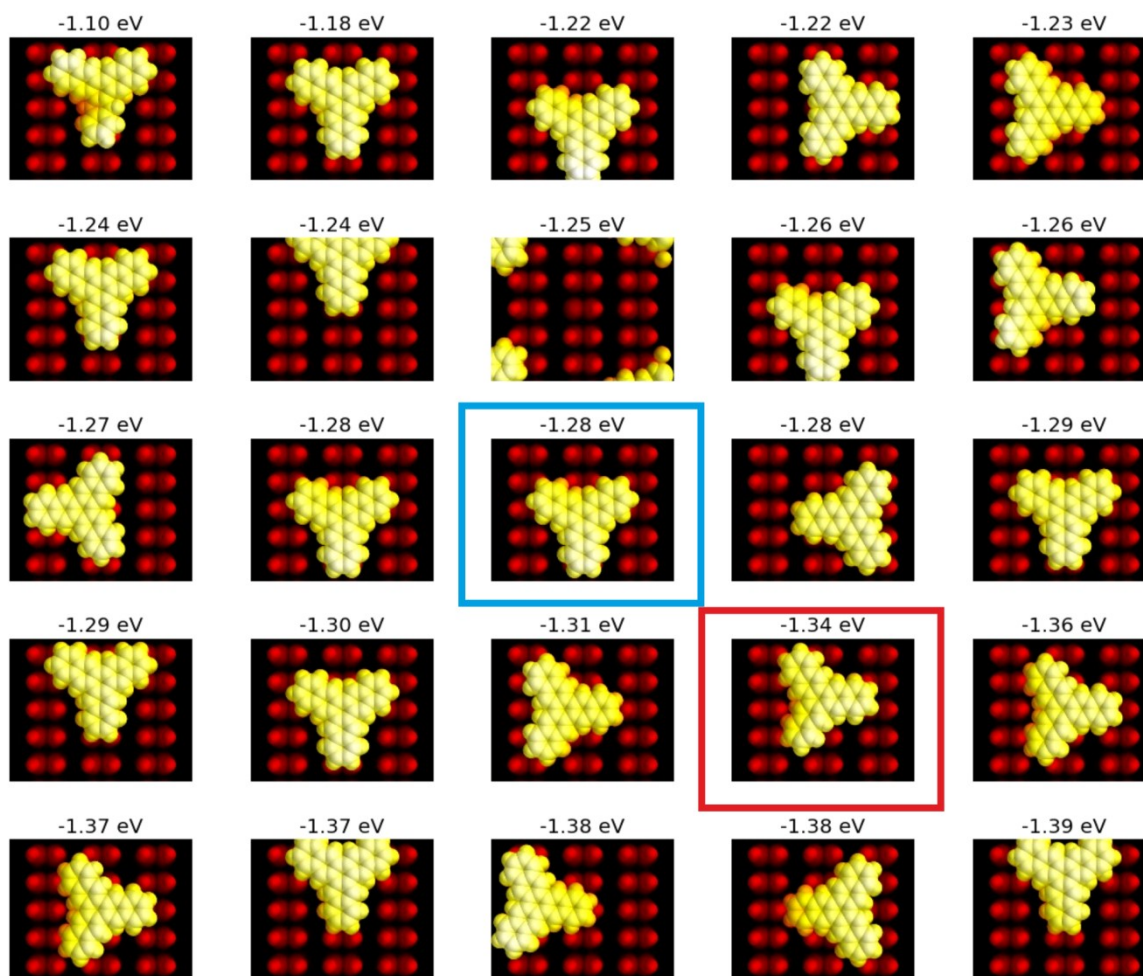


Figure S1. All configurations considered in the study. Atoms are displayed as balls using van der Waals radii of respective elements. The color codes the out of plane altitude from black indicating most deeply located structures up to white coding the parts exhibiting the highest altitude. The structure, in which chemical bond is formed between the molecule and the surface is shown in the upper left-hand side corner. The adsorption energies are displayed above the respective image. The geometries 1 and 2 discussed in the main text of the manuscript are marked with blue and red rectangles, respectively.