Theoretical study of ptcda molecules adsorbed on InSb(001) surface

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Experimental STM studies of PTCDA molecules deposited on InSb(001) surface with c(8x2) reconstruction resulted in interesting pictures of molecular chains.
Their arrangement and orientation of individual molecules was unclear. To solve this problem, numerous DFT searches and optimizations were performed.
They enabled successful description of observed adsorption sites.
The theoretical work unveiled also an interesing interplay between dimensions of the molecule and surface geometry, which leads to highly anisotropic diffusion. The process is controlled by a pattern of chemical bond formation sites.