

Electronic rearrangements during the inversion of lead phthalocyanine

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Application of metal phthalocyanines (MPc's) as molecular switches is based on the possibility to control the conformational changes of the adsorbed molecules as well as their electronic and magnetic states. Particularly, PbPc can adsorb on a range of different substrates in two orientations due to its shuttlecock shape: either having the central metal atom towards (PbPc \downarrow) or away from (PbPc \uparrow) the surface [1-2]. The reversible switching between these configurations can be triggered by small but energetic nanomechanical motions. As a result, one can use the effect for constructing molecular memories and sensors at the nanoscale.

Here we present work devoted to studying of the mechanism of PbPc inversion from the bonding evolution theory standpoint, enabling one to monitor the electronic structure rearrangements in the course of elementary reaction [3]. It was found that reorganization of Pb's ELF basins with pronounced role of core ones is the basis of the catastrophes identified, whereas ELF basins belonging to other atoms are almost not involved in the electronic structure changing [4]. The results obtained provide the new topological picture of processes underlying the conformational transitions of shuttlecock shaped MPc's adsorbed on surfaces.

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