新学術領域「コンピューティクスによる物質デザイン：複合相関と非平衡ダイナミクス」
計画研究／公募研究「ｘｘｘｘ」

Hydrazine adsorption conformations on metal surfaces

Mohammad Kemal Agusta, Hiroshi Nakanishi, Wilson Algerico Diño, Hideaki Kasai
Department of Applied Physics, Osaka University, Suita, Osaka 565-0871

Study of hydrazine adsorption on metal surface is important from both scientific and applicative point of views. The system could serve as a model for adsorption of species with lone-pair characteristic and structural conformations. It is also important in providing insights into the design of a better catalyst for the direct hydrazine fuel-cell technology.

Being viewed as a joint of two NH_2 groups via N – N sigma-bond, hydrazine possesses structural conformations due to internal rotation around its N – N axis. Three critical conformations are named by anti, gauche and cis. It has been established that gauche conformation is the most stable conformation for the molecule in the gas-phase. The minimization of the lone-pair repulsion is the mechanism behind the preference of this conformation.

Upon adsorption on surface, the first-order charge transfer mechanism stabilizes anti over gauche-conformation. This mechanism derives bonding and anti-bonding states between surface and adsorbate. The occupancy of the anti-bonding states determines the stability of the bonding and also the conformations. In addition to that, the adsorption also involves formation of dative type of bonding that corresponds to the second-order charge transfer.

Furthermore, a model based on perturbative interaction between surface d and sp-states with adsorbate frontier orbitals is used to predict the trend of adsorption energy. Analysis reveals strong repulsive characteristic in the interaction and elucidates the role of the sp-states in the bonding formation.

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