Chinese Journal of Chemistry 2005 23 (11): 1479-1482 ISSN: 0567-7351 CN: 31-1320/06

Full Papers

量子化学研究**NO**在铜负载金红石表面降解反应

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收稿日期 2005-4-30 修回日期 2005-7-15 网络版发布日期 接受日期

摘要 应用密度泛函方法结合嵌入簇模型对NO在铜负载金红石表面的吸附与降解进行了研究，计算结果表明NO分子解离以氧端吸附形成N_2O中间体然后解离N_2和 O_2.过程，另一条途径为NO双分子直接解离。通过能量学计算揭示了生成N_2O中间体对降解NO更为有利。

关键词 密度泛函方法, Cu/TiO_2, 嵌入簇模型

分类号

Reduction of Nitric Oxide over Rutile-supported Cu Surfaces: A Quantum Chemical Study

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Abstract The adsorption and decomposition of NO on the stoichiometric rutile-supported Cu surfaces have been studied by means of density functional calculations with an embedded cluster model. The calculation results indicate that NO is favorably adsorbed as O-down and could easily attach another NO molecule to form N_2O intermediate or directly be dissociated into N_2 and O_2. On the basis of the calculated energetics, possible mechanism of NO decomposition reaction has been proposed.

Key words DFT Cu/TiO_2 embedded cluster model

DOI:

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