Joint CQSE and CASTS Seminar

Weekly Seminar
Mar. 30, 2012 (Friday)

TIME Mar. 30, 14:30 ~ 15:30

TITLE First Principles Calculations to Study the Decomposition Reactions of NO_x and CO_2 Gases and Ammonia synthesis on the Transition-Metal Surfaces

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Abstract

The calculations of the mechanism of decomposition of CO_2 and NO_2 on the Fe(111) surface are reported, we found that the Fe(111) surface exhibits a large catalytic activity to decompose CO_2 and NO_2. The rate coefficients for the dissociative adsorption of CO_2 and NO_2 have been predicted with variational TST and RRKM theories, and the interaction between adsorbate and substrate was subjected to a detailed electronic analysis. This information about the reaction mechanism, the catalytic activity of various surface sites, and the relevance of the surface structure, would be laborious to obtain by experimental measurements, indicating that periodic DFT calculations might play a vital role in the rational design of improved catalytic surfaces for the dissociation of CO_2 and/or NO_2. To the best of our knowledge, this is the first time theoretical approach, and our work is expected to be welcomed by many surface chemists, spectroscopists and experimental scientists.