

Infrared Spectroscopy of Ammonia on Iron: Thermal Stability and the Influence of Potassium

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Abstract

We report on reflection–absorption infrared spectroscopy investigations, supported by first-principles density functional theory, into the surface chemistry of NH₃ on Fe{111}. Ammonia is found to adsorb intact at low temperature and predominantly to desorb intact at around room temperature. Some of the adsorbed molecules dissociate if the surface is held at temperatures a little below the desorption temperature, transiently producing NH₂ (directly observed) and ultimately NH and/or N (both inferred). Preadsorbed potassium is found to substantially weaken the interaction of ammonia with the surface, to induce a change in the ammonia adsorption geometry, and to promote both ammonia desorption and dissociation.