

Ferroelectric Surface Chemistry: First-Principle Study of NO_x Decomposition

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NO_x molecules are critical and regulated air pollutants produced during automotive combustion. As part of long-term effort to design viable catalysts for NO_x decomposition that operate at higher temperatures, and thus would allow for greater fuel efficiency, we are studying the basic science of NO_x chemistry on ferroelectric perovskite surfaces. Changing the direction of the ferroelectric polarization can modify surface electronic properties and thus can lead, in principle, to switchable surface chemistry. Here, we begin with the question of how NO and NO_2 molecules behave on the polar (001) surfaces of ferroelectric PbTiO_3 as function of ferroelectric polarization, surface stoichiometry, and various molecular or dissociated binding modes. We will discuss our calculated polarization and coverage dependences based on the electronic structure of the surface system.

This work is funded by the Toyota Motor Engineering and Manufacturing, North America, Inc.