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Ferroelectric Surface Chemistry: FIrst-principle study of NOx Decomposition[1] ARVIN KAKEKHANI, SOHRAB ISMAIL-BEIGI, Yale University, SOHRAB ISMAIL-BEIGI'S TEAM — NOx molecules are critical and regulated air pollutants produced during automotive combustion. As part of a long-term effort to design viable catalysts for NOx decomposition that operate at higher temperatures and thus would allow for greater fuel efficiency, we are studying NOx chemistry on ferroelectric perovskite surfaces. Changing the direction of the ferroelectric polarization can modify surface properties and thus can lead to switchable surface chemistry. We will discuss our results for NO and NO2 on the polar (001) surfaces of PbTiO3 as function of ferroelectric polarization, surface stoichiometry, and various molecular or dissociated binding modes.

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