

Abstract Submitted  
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**NO<sub>x</sub> Direct Decomposition: Potentially Enhanced Thermodynamics and Kinetics on Chemically Modified Ferroelectric Surfaces<sup>1</sup>**  
ARVIN KAKEKHANI, SOHRAB ISMAIL-BEIGI, Yale University — NO<sub>x</sub> are regulated pollutants produced during automotive combustion. As part of an effort to design catalysts for NO<sub>x</sub> decomposition that operate in oxygen rich environment and permit greater fuel efficiency, we study chemistry of NO<sub>x</sub> on (001) ferroelectric surfaces. Changing the polarization at such surfaces modifies electronic properties and leads to switchable surface chemistry. Using first principles theory, our previous work has shown that addition of catalytic RuO<sub>2</sub> monolayer on ferroelectric PbTiO<sub>3</sub> surface makes direct decomposition of NO thermodynamically favorable for one polarization. Furthermore, the usual problem of blockage of catalytic sites by strong oxygen binding is overcome by flipping polarization that helps desorb the oxygen. We describe a thermodynamic cycle for direct NO decomposition followed by desorption of N<sub>2</sub> and O<sub>2</sub>. We provide energy barriers and transition states for key steps of the cycle as well as describing their dependence on polarization direction. We end by pointing out how a switchable order parameter of substrate, in this case ferroelectric polarization, allows us to break away from some standard compromises for catalyst design (e.g. the Sabatier principle). This enlarges the set of potentially catalytic metals.

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