A Potentially New Window towards Catalysis: Polarization Dependent Chemistry on Ferroelectric Surfaces

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The fact that a bulk material has an order parameter raises an interesting question as to how its surface chemistry can be affected by the order parameter. We use DFT methods to explore the possibility of flippable surface chemistry by switching the polarization of a ferroelectric substrate. One specific practical application is to potentially use ferroelectric surfaces for effective reduction of NO_x molecules (which are environmental pollutants) in oxygen rich environments. The difficulty of catalyzing NO_x reduction is a key problem with current automotive catalysts which force lower oxygen content and thus lower fuel efficiency.

In addition to exploring the effect of order parameter of the substrate, we show how depositing a monolayer of an active transition metal oxide, in this case RuO_2, can enhance desirable chemical reactions on the surface. This approach provides an additional degree of freedom in controlling surface chemistry which can be exploited to expand the types of transition metals that can be used as effective catalysts.

We present results for polarization dependent binding and dissociation energies of N_2, O_2, and NO molecules, atomic N and O, and we describe how this leads to new types of proposed catalytic pathways for NO_x reduction.