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Computational Database of Metal-Oxide Surface Reactivities for Catalyst Design[1] MICHAL BAJDICH, ALEKSANDRA VOJVODIC, JENS K. NØRSKOV, SLAC National Accelerator Laboratory — We study surface reactivity of low index facets of MO, MO2 and ABO3 oxide groups using small atoms and molecules (O, OH, CO, NO, CH3, NH3). The computed database of adsorption and activation energies will be used to identify possible correlations with other quantities such as surface energies or electronic structure in order to establish scaling relations for future high-throughput screening efforts. A comparison will be made between DFT functionals of various levels of accuracy, e.g., GGA, GGA+U, GGA+vdW and GGA-hybrid, meta-GGA and hybrid meta-GGA, and compared to available experiments. This effort is part of the "Predictive Theory of Transition Metal Oxide Catalysis" funded through the DOE Materials Genome Project.

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