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First-principles design of a dynamically tunable catalyst for CO_2 capture and conversion BABATUNDE ALAWODE, ALEXIE KOLPAK, Massachusetts Institute of Technology — Due to its role in climate change, there is great interest in finding ways to take advantage of the vast amount of waste CO_2 we produce by its conversion to useful substances. This approach is currently impractical due to the high temperatures and pressures generally required for the synthesis of compounds using CO_2 as a precursor. To make direct CO_2 capture and conversion economically viable, new materials able to catalyze the conversion reactions at significantly milder conditions will be essential. In this work, we use DFT computations to design a dynamically tunable ferroelectric oxide-supported thin film catalyst that can capture CO_2 directly from the emission stream and convert it into methanol. One promising candidate for a dynamically tunable catalyst of this type is $Zn_xO_y/PbTiO_3$. We demonstrate that switching the polarization of the ferroelectric substrate substantially changes the surface atomic and electronic properties of the heterostructure, thereby alternately encouraging strong CO_2 adsorption and desorbing the products. Our approach may lead not only to new technologies for reducing emissions, but also to novel catalysts that could decrease energy consumption for industrial-scale synthetic processes.

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