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Polarization dependence of carbon dioxide dissociation on palladium supported on ferroelectrics¹ SEUNGCHUL KIM, ANDREW M. RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania — Using density functional theory (DFT) calculations, we investigate the effect of polarization direction on the catalytic activity of palladium supported on ferroelectrics. It is calculated how the energy barriers of the carbon dioxide (CO_2) dissociation process into carbon monoxide (CO) and oxygen (O) are changed for positively and negatively polarized ferroelectric lithium niobate (LiNbO_3) surfaces. In this study, the LiNbO_3 surfaces are passivated by ions, which is thermodynamically favored for a wide range of chemical potentials. Multiple possible CO_2 dissociation paths and their energy barriers are presented. We also perform a detailed analysis of electronic structure to explain differences in the reaction process on the two surfaces.

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