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Stability Analysis of Catalytic Compounds Using Computational Simulations RICHARD KYUNG, Choice Research Group, KWANGJIN AN, GABOR A. SOMORJAI, Department of Chemistry, University of California, Berkeley — The ultimate goal of the research on the energy is to actualize green energy and increase its efficiency, achieving better selectivity and molecular stability of the desired product. Metal nanoparticles and oxide supports can increase catalytic selectivity to obtain desirable products. In this paper, the chemical catalytic efficiency and physical activities of proposed metal oxide compounds are modeled and analyzed using computational simulations. The compounds' mechanical repulsive forces, electron structures, and bond strengths are explained. In order to model the electron properties of the compounds, the computational and numerical DFT methods are used. To check the mechanical stability and convergence of the solutions, energy(kcal/mol) versus computational steps(N) curves for each metal compounds are presented. Also, the theoretical structure of each feasible catalytic Platinum(Pt) compound has been studied in this project. Based on the predicted physical stability of each molecule, the compound that can be used most efficiently to catalyze the reaction for the green energy can be determined.

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