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Stability Analysis of Compounds Using the Computational and Physical Mechanics MYUNGJIN LEE, RICHARD WU, MINJI CHUNG, Choice Research Group — The physical activities and chemical catalytic efficiency of proposed metal oxide compounds are modeled and explained based on the compounds' mechanical repulsive forces, electron structures, and bond strengths. The ultimate goal of the research is to actualize green energy, achieving better selectivity and physical stability of the desired product molecule. In order to model the electron properties of the compounds, the computational and numerical methods are used. To check the stability and convergence of the solutions, computational steps(N) versus energy(kcal/mol) curves for each metal compounds are presented. The theoretical structure of each feasible catalytic palladium 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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