Abstract Submitted
for the NWS16 Meeting of
The American Physical Society

Stability Analysis of Metal Oxide Compounds Used in Combustion Reaction by Computational and Physical Method JAEWOO KIM, BYUL SOHN, JAEWON LIM, Choice Research Group — The theoretical structure of feasible catalytic compound is presented in this study. The physical activity and chemical stability of catalytic compounds are proposed after modeling and analyzing the molecule based on the compounds electron structures, and bond lengths and bond strengths. The ultimate goal of presented research is to achieve better selectivity in producing green energy. Also convergence test of the proposed molecules is carried out to determine the stability of the metal oxides. Numerical and computational methods are used in order to model the electron properties of the compounds. Computational steps(N) versus energy(kcal/mol) curves for each metal compounds are presented to check the stability and convergence of the molecules.

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Date submitted: 26 Apr 2016 Electronic form version 1.4