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**Computational and Physical Analysis of Catalytic Compounds**

RICHARD WU, JUNG JAE SOHN, RICHARD KYUNG, Choice Research Group — Nanoparticles exhibit unique physical and chemical properties depending on their geometrical properties. For this reason, synthesis of nanoparticles with controlled shape and size is important to use their unique properties. Catalyst supports are usually made of high-surface-area porous oxides or carbon nanomaterials. These support materials stabilize metal catalysts against sintering at high reaction temperatures. Many studies have demonstrated large enhancements of catalytic behavior due to the role of the oxide-metal interface. In this paper, the catalyzing ability of supported nano metal oxides, such as silicon oxide and titanium oxide compounds as catalysts have been analyzed using computational chemistry method. Computational programs such as Gamess and Chemcraft has been used in an effort to compute the efficiencies of catalytic compounds, and bonding energy changes during the optimization convergence. The result illustrates how the metal oxides stabilize and the steps that it takes. The graph of the energy computation step(N) versus energy(kcal/mol) curve shows that the energy of the titania converges faster at the 7th iteration calculation, whereas the silica converges at the 9th iteration calculation.

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