

Theoretical Studies for Explaining Dynamic Metal-Polymer Interaction for the Design of Chemoselective and Long-lived Hydrogenation Catalysts

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Recently, the unique catalytic properties of metal particles supported on a thermochemically stable but "soft" polymer showing substantial mobility under the reaction conditions were demonstrated. Here, we tried to deeply understand the system using molecular dynamics (MD) and density functional theory (DFT).

First, dynamic interaction between metal and polymer was investigated based on MD. Force field parameters were tuned to reproduce glass transition temperature ( $T_g$ ) of polymers and binding energy between metal and polymer. Then, it was figured out the monolayer of polymer covered the entire surface of Pd particles near  $T_g$  (~353K).

Finally, catalytic selectivities were studied based on DFT. The materials showed high selectivity for acetylene partial hydrogenation versus ethylene, industrially important for the downstream processing of ethylene produced by steam cracking. Thermodynamics from DFT well explained this results.