Catalytic CO_2 Hydrogenation to Formic Acid over Defect Graphene Coordinated Pd-Ni Nanoparticles

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Pd-Ni alloy has been reported to bring a brought a significant enhancement in catalytic monometallic Pd catalyst for the CO_2 hydrogenation to formic acid.a By means of periodic density functional theory calculations, we have investigated the adsorption behaviors of CO_2, formate intermediate (HCOO) and formic acid (HCOOH) over pure Pd an Pd-Ni alloyed clusters on defect graphene support in various conditions. According to lowest free energy pathway in our results, we found that The dissociation of HCOO* to H* + CO_2* over Pd cluster is thermodynamically favorable but becomes endergonic on bimetallic system, indicating alloying Pd with Ni could stabilized the HCOO* and hinder the revise reaction to H* + CO_2*.

References

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