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Onboard Catalysis of Formic Acid for Hydrogen Fueled Vehicles
ALTAF KARIM, MUHAMMAD MAMOOR, COMSATS Institute of Information Technology Islamabad — Metal hydrides are used as a medium of hydrogen storage in hydrogen powered vehicles. Such hydride materials cannot store hydrogen more than 10 wt%. The bottleneck in this issue is the reversible storage of hydrogen at ambient temperature and pressure. Alternatively formic acid is becoming more popular medium for the onboard hydrogen production for these vehicles. Its decomposition on metal surfaces and nanostructures is considered to be a potential method to produce CO-free hydrogen at near ambient temperatures. We applied Density Functional Theory (DFT) based Kinetic Monte Carlo (KMC) simulations as our tool to study the reaction kinetics of hydrogen production from formic acid on different catalytic surfaces and nano structures (Au, Pd, Rh, Pt). Our results show that nanostructures and artificially engineered bimetallic catalysts give higher rate of hydrogen production then their monometallic counter parts under various temperature and pressure conditions.

Altaf Karim
COMSATS Institute of Information Technology Islamabad

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