Atomically Dispersed Electrocatalysts for Low Temperature Fuel Cell and Water Electrolysis

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It is of great importance to reduce the amount of noble metals in the chemical industry. In this sense, single atom or atomically dispersed catalysts have attracted much attention due to high metal utilization and unique catalytic property. In this presentation, we will show a combination of density functional theory (DFT) and experimental approaches to explore the stability and electrocatalyic activity of a wide range of metal single atoms on a TiC support. We also tuned and enhanced the activity of Fe-N-C, atomically dispersed electrocatalyst, by givign the effect of electron withdrawing/donating functionalities.