Hydrogen Spillover and Storage on Graphene by Single-Site Ti Catalysts

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Abstract

Single-site metal catalysts are separately placed on a carrier for stably storing the reduced reactant, which has promising activity and selectivity for various current and emerging industrial processes. The phenomenon of hydrogen spillover and storage of single-site metal catalysts has been clarified theoretically and experimentally, but due to its complex nanoscale structure, the understanding of inert carbon supports is still poorly understood [1-3]. Here, we atomically deposit titanium atoms on epitaxial graphene to anchor Ti atoms into the graphene hollow sites to eliminate the influence of electronic and surface chemical effects on the catalytic performance of hydrogen molecules at room temperature and moderate pressure. Our combined *in situ* angle-resolved photoemission spectroscopy (ARPES), ambient pressure X-ray photoemission spectroscopy (APXPS) and X-ray absorption spectroscopy (XAS) studies reveal trends between hydrogen dissociation to form a stable H-C bond on graphene, thereby opening the band-gap. Our results also demonstrate how simple catalyst process can be used to create hydrogenation process, which provides a strategy for rational design of carbon-supported catalysts.

Keywords **– single-site metal catalyst, hydrogen spillover, angle-resolved photoemission spectroscopy (ARPES), ambient pressure X-ray photoemission spectroscopy (APXPS) and X-ray absorption spectroscopy (XAS)**

References

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