

Department of Physics, National Central University



Colloquium

Study of Hydrogen Spillover and Storage on Ti Loaded Graphene with Synchrotron Radiation Techniques

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Abstract:

Hydrogen spillover and storage for single-site metal catalysts, including single-atom catalysts (SACs) and single nanocluster catalysts, have been elucidated for various supports but remain poorly understood for inert carbon supports. To have a deeper understanding of such behavior, we utilized synchrotron-radiation-based methods to investigate the role of single-site Ti catalysts on graphene for hydrogen spillover and storage. Our in situ angle-resolved photoemission spectra results demonstrate a band gap opening, and X-ray absorption spectra reveal the formation of C-H bonds, both indicating partial graphene hydrogenation. With increasing Ti deposition and H₂ exposure, the Ti atoms tend to aggregate to form nanocluster catalysts and yield 13.5% sp³-hybridized carbon atoms corresponding to a hydrogen-storage capacity of 1.11 wt %. Our results demonstrate how a simple spillover process at Ti SACs can lead to covalent hydrogen bonding on graphene, thereby providing a strategy for the rational design of carbon-supported single-site catalysts.