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In situ Raman Evidence for Reversible Room-Temperature Hydrogenation in Pt-doped Carbons<sup>1</sup> XIAOMING LIU, PSU Materials Research Laboratory, YOUJIAN TANG, ENSHI XU, PSU Department of Physics, THOMAS FITZGIBBONS, PSU Department of Chemistry, HUAN-HSIUNG TSENG, MING-SHENG YU, CHENG-SI TSAO, Taiwan Institute of Nuclear Energy Research, JOHN BADDING, PSU Department of Chemistry, VINCENT CRESPI, PSU Department of Physics, ANGELA LUEKING, PSU Department of Chemical Engineering and EMS Energy Institute, ANGELA D. LUEKING TEAM, JOHN V. BADDING TEAM, VINCENT H. CRESPI TEAM, CHENG-SI TSAO COL-LABORATION — Atomic hydrogen spillover was investigated by in situ Raman spectroscopy and density functional theory. In the presence of Pt nanoparticles, modes related to Basal plain hydrogenation were observed for activated carbon and graphene, respectively, during Raman measurements in 100 bar H2. The modes were absent when Pt, carbon, or H2 were omitted from the experiment. Substituting H2 with D2 led to the expected isotopic shift for a hydrogen-dominated vibrational mode. The mode disappeared and reappeared over several cycles of exposure to H2 or He at room temperature, consistent with room-temperature reversibility of H chemisorbed to the activated carbon in the presence of Pt nanoparticles. Reversibility apparently arises from a facilitated transition of H from a chemisorbed state to a more mobile physisorbed state, followed by recombination and release. Reversibility for Pt/graphene was much less pronounced, suggesting that structural heterogeneities in the sample carbon support and/or catalyst-carbon contact are important factors.

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