Substrate enhanced stability of hydrogen adsorption complexes on graphene on Ir(111)

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We present temperature programmed desorption (TPD) measurements investigating the interaction of hydrogen with graphene supported on an Ir(111) substrate. These experiments demonstrate how the substrate influences the reactivity of graphene towards atomic hydrogen, as well as the stability of the resulting hydrogenated graphene compounds. The presented data reveal a distinctively different behavior for hydrogenated graphene on an Ir(111) substrate as compared to hydrogenated graphite.

Figure 1 shows a TPD spectra for D_2 desorbing from graphene on an Ir(111) substrate for a series of relative D coverages with respect to that at saturation. A distinct asymmetric peak is evident in the spectra. Analysis of the spectra revealed that the barrier to D_2 desorption is significantly larger than what is found for the desorption of D_2 from graphite [1]. It has previously been suggested that hydrogen chemisorbed on graphene on an Ir(111) substrate form a graphane-like structure [2]. Such a graphane model can successfully explain the observed enhanced stability of the hydrogen adsorbates.

It was also found that the absolute coverage of D adsorbed on graphene on an Ir(111) substrate at saturation is independent of the kinetic energy of the impinging D atoms. This is in contrast to the behavior observed for HOPG, where the absolute coverage at saturation is reduced for lower D beam temperatures. Such a temperature dependence is directly related to the existence of adsorption barriers, which are a consequence of surface reconstruction during the C-H bond formation [3]. These adsorption barriers are most likely modified by the presence of the underlying Ir(111) substrate resulting in different kinetics for hydrogenation than those observed for HOPG. Hence, even though graphene on Ir(111) exhibits electronic properties that are essentially unchanged from those for free standing graphene, the chemical properties of graphene are observed to be severely modified by the underlying substrate.

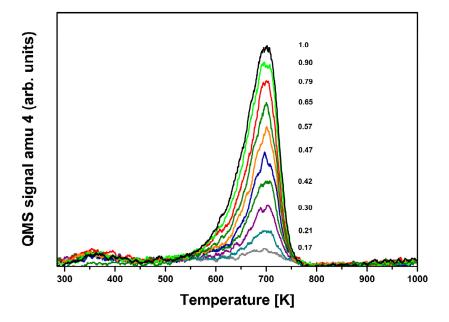


Figure 1 TPD spectra of D_2 desorbing from graphene on an Ir(111) substrate following exposure to atomic D. The employed temperature ramp was 1 K/s. The individual traces are labeled with coverage relative to that achieved at saturation.

References:

- 1. Zecho, T., et al., *Adsorption of hydrogen and deuterium atoms on the (0001) graphite surface.* Journal of Chemical Physics, 2002. **117**(18): p. 8486-8492.
- 2. Balog, R., et al., *Bandgap opening in graphene induced by patterned hydrogen adsorption*. Nature Materials, 2010. **9**(4): p. 315-319.
- 3. Sha, X.W. and B. Jackson, *First-principles study of the structural and energetic properties of H atoms on a graphite (0001) surface*. Surface Science, 2002. **496**(3): p. 318-330.