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**Excited Carriers Relaxation and Hydrogen Dissociation on Hydrogenated Graphene: A Theory** JUNHYEOK BANG,

Y.Y. SUN, D. WEST, S.B. ZHANG, Department of Physics, RPI, Troy, New York 12180, USA, S. MENG, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, Z.G. WANG, F. GAO, PNNL, Richland, Washington 99352, USA — Using *ab initio* molecular dynamics coupled with time-dependent density functional theory (TDDFT), we show that the energy transfer of photo-excited carriers into atomic kinetic energy on hydrogenated graphene depends sensitively on the surface H coverage. Here, the energy transfer rate plays a crucial role in the determination of the H dissociation dynamics from graphene. In the low density “isolated” hydrogen atom limit, the energy transfer is significantly suppressed 80 fs after the excitation. Thus, it is difficult to dissociate hydrogen due to the faster energy dissipation from H into carbon backbone, despite that initially the H kinetic energy had increased to around 1.5 eV and the C-H bondlength had stretched to 2.4 Å. In sharp contrast, at the high-density graphane limit, an efficient energy transfer channel is established when the C-H bondlength exceeds 1.4 Å. A fraction of the H readily dissociates within 15 fs. This is because ionized H forms a charged layer that expels, and as such accelerates the H ions with higher initial thermal velocities flying away. Our study thus reveals the importance of performing TDDFT calculations for excited carrier dynamics as from the widely adopted ground-state or constrained DFT dynamics one would expect the C-H bonds in graphane to be significantly stronger, due to full surface passivation, than that of isolated

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