Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Photo-exfoliation of graphene from graphite: An \textit{ab initio} study$^1$
HONG ZHANG, Sichuan University, YOSHIYUKI MIYAMOTO, NEC, DAVID TOMÁNEK, Michigan State University — Mass production of high-quality graphene monolayers is an essential prerequisite for producing graphene devices [1]. Flaws of current synthesis techniques, such as chemical exfoliation combined with sonication [2] are remaining contaminants, and CVD synthesis [3] suffers from the influence of the substrate [3]. The best quality graphene monolayers are still obtained using the scotch-tape technique [1], which is ill-suited for mass production. By performing \textit{ab initio} TDDFT-MD calculations, we have identified irradiation by ultra-short laser pulses as a suitable technique to produce graphene monolayers by photo-exfoliating graphite without the above drawbacks. Our simulations indicate that exposing graphite to 800 nm laser pulses with a suitable pulse shape and intensity may cause detachment of single graphene layers due to a non-equilibrium charge redistribution in a vibrationally cold substrate [4]


$^1$Supported by NSF NSEC grant EEC-425826.