

Abstract Submitted
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Photo-exfoliation of graphene from graphite: An *ab initio* study¹

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 *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] K. S. Novoselov *et al.*, Science **306**, 666 (2004), and supporting mat.

[2] X. Li *et al.*, Science **319**, 1229 (2008).

[3] A. Reina *et al.*, Nano Lett. **9**, 30 (2008); X. Li *et al.*, Science **324**, 1312 (2009).

[4] Y. Miyamoto, H. Zhang, and D. Tománek, submitted.

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