Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Time-Dependent Density Functional Theory Applied for Pulse Laser Shot: Criterion of the Numerical Stability[1] YOSHIYUKI MIYAMOTO, CREST-JST, Nano Electronics Res. Labs. NEC, HONG ZHANG, Sichuan University — In this talk, applications of TDDFT [1] for irradiation of pulse laser to materials and subsequent structural change are shown. Contrary to the pioneering works [2-3], we present a way of judging numerical stability which can be confirmed by the energy conservation rule. The conserved quantity is the DFT total energy plus kinetic energy of ions minus work done by the pulse shot [4], which can simply be demonstrated with use of adiabatic exchange-correlation functional and time-varying electric field generated by a time-varying fictitious charge. As an example, structural change on graphite surface induced by pulse laser shot is demonstrated with use of 10-layer AB- stacked slab model. After irradiating laser shot with wavelength of 800 nm, pulse width of 50 fs, and a power about 90 mJ/cm^2 per pulse, the top graphene monolayer spontaneously leaves while other layers remain.

[1] E. Runge and E. K. U. Gross, Phys. Rev. Lett, **52**, 997 (1984).
[2] K. Yabana and G. F. Bertsch, Phys. Rev. B**54**, 4484 (1996)
[3] A. Castro et al., Eur. Phys. J. D**28**, 211 (2004).
[4] Y. Miyamoto and H. Zhang, Phys. Rev. B**77**,165123 (2008).

[1]All calculations were performed by using the Earth Simulator.

Yoshiyuki Miyamoto
CREST-JST, Nano Electronics Res. Labs. NEC

Date submitted: 07 Nov 2008 Electronic form version 1.4