# Electron-ion relaxation in Al nanoparticles: non-adiabatic wave packet molecular dynamics

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Fast progress in nanoplasmonics determined strict requirements for the synthesis of nanoparticles with specified geometrical properties. Reshaping under femtosecond laser pulses has become a promising technique for such task [1]. Ultrashort laser impulses of high intensity excite electron subsystem which then transfers energy to ions via electron-ion relaxation and transforms the nanoparticle into so-called warm-dense matter state (WDM). WDM remains the subject of great scientific interest from both experimental and theoretical point of view.

Here by means of eFF potential [2,3] we apply non-adiabatic wave packet molecular dynamics (WPMD) approach to calculate the structural evolution of fs-laser irradiated aluminum nanoparticles during the first picoseconds after irradiation. The eFF potential provides the combination of particle dynamics for ions with wave packet dynamics representing electrons as floating Gaussians. Unlike the more complex antisymmetrized approximation [4], interactions between electrons in the eFF model are restricted to pairwise components only and the total energy of the system is evaluated as in classical force field methods. eFF does not utilize Born-Oppenheimer approximation allowing us to model structural properties and non-adiabatic electron dynamics, such as electron-ion relaxation, within a single framework. Our results demonstrate a significant influence of the electronic pressure [5] on the processes of thermalization, melting and acoustic vibrations launching in metal nanoparticles under fs-laser irradiation.

## REFERENCES

[1] González-Rubio G. et al 2017 Science 358, 640–644
[2] Su J T and Goddard W A 2007 Phys. Rev. Lett. 99 185003
[3] Jaramillo-Botero A et al 2011 J. Comp. Chem. 32 497–512
[4] Morozov I and Valuev I 2012 Contrib. Plasma Phys. 52 140–144
[5] Stegailov V and Zhilyaev P 2015 Contrib. Plasma Phys. 55, No. 2-3, 164 – 171