



Tuesday 7<sup>th</sup> of December 2021 at 15:00 in room C  
of the Department of Chemical Sciences

## Prof. Tatiana Itina

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Will give the talk:

### **Modeling of laser-assisted nanoparticle formation, sintering and fragmentation**

The use of various laser systems is extremely promising for nanoparticle formation, sintering and fragmentation because of the possibilities of control over their size, composition, and properties. In particular, short and ultra-short laser pulses are known to be efficient for the synthesis of small and chemically clean nanoparticles in liquids, as well as for the formation of various nano-hybrids and nanoalloys of normally immiscible materials.

Laser interactions commonly involve excitation of the electronic sub-system followed by energy relaxation, material heating, phase transitions, emission of various species. Additionally, thermoplasmonic effects, reshaping, internal atomic diffusion, mixing, fragmentation, or sintering may take place in laser interaction with nano-objects. In this talk, attention will be focused on multi-physical and multi-scale models simulating not only laser ablation but also size-dependent nanoparticle absorption and local field enhancement, photo-induced free carrier generation, plasmon-assisted electron emission, and heat transfer. Then, several results of a series of atomistic molecular dynamics simulations will be presented. The role of laser parameters, of nanoparticle size, temperature, cohesive energy, atomic mass, and initial composition will be analyzed.