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# Modeling Nanoparticle Synthesis via Laser Ablation for Advanced Applications

Tatiana Itina

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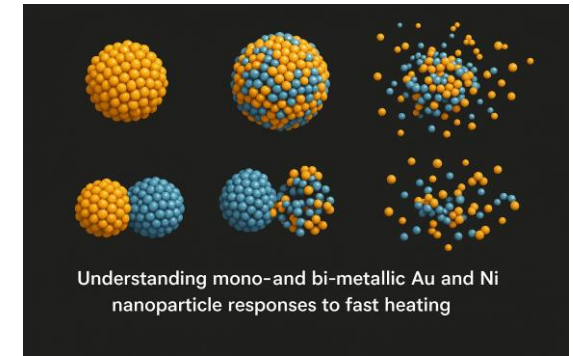
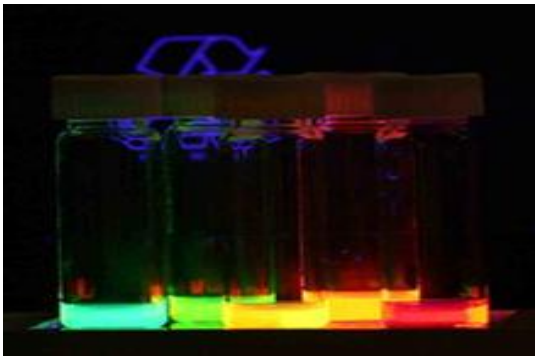


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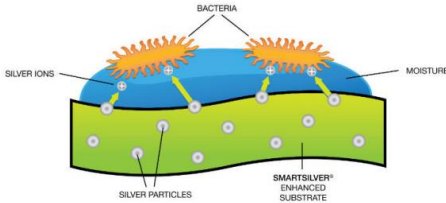
# Modeling Nanoparticle Synthesis via Laser Ablation for Advanced Applications

Tatiana E. ITINA

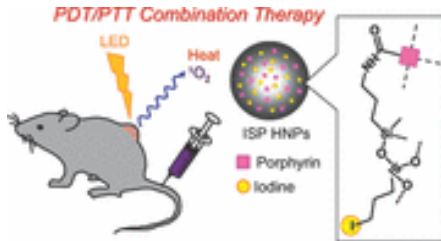
Lab. Hubert Curien, UMR CNRS 5516, UJM, Campus Manufacture, 42000 St-Etienne, France



# Applications of NPs



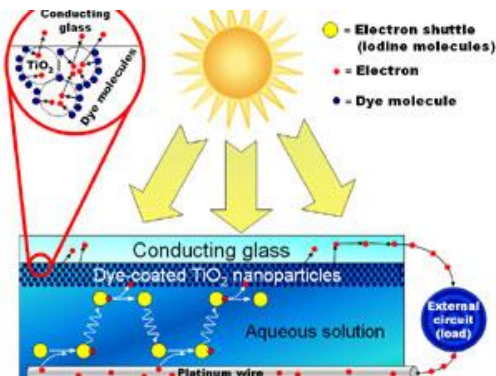
<http://www.nanowerk.com/spotlight/spotid=19451.php>



Hayashi et al.



DOI: 10.1039/C1CP22048A



Agrios, Northwestern University

**Textiles:** anti-bacterial properties, order elimination, self-cleaning, UV protection, fireproof, release of active agents, luminescence, durability, heat, antistatic, ... (Ag, ZnO, TiO<sub>2</sub>, SiO<sub>2</sub>, CNT, etc.)

**Health:** tumor treatments, imaging, sensors, SPR, etc.. (colloidal/gas Au, Ag, Si, etc.)

**Chemistry, catalysis, cosmetics:**

(colloidal metal NPs, TiO<sub>2</sub>, nanoalloys, ex: AgPd, etc...), etc.

**Food:** flavor modifications, water treatment (Ag, nanocomposites: Cu, Ni, No) can be dangerous

**Energy** (sollar cells), **transport** (cooling, nanofluidics, anti-wetting, nanocomposites, etc.)

**Airspace industry, buildings, furniture,** etc.

# Advantages of NP Synthesis by Laser Ablation

Chemical Methods

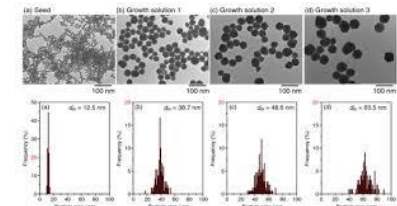
Physical Methods

Biological Methods

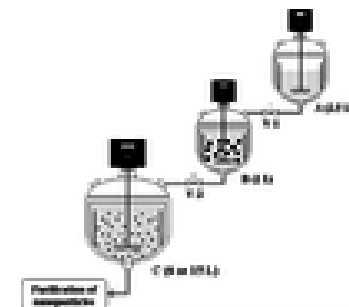
## 1. Green methods



## 2. Better control over properties



## 3. Scaling-up possibility



AgNPs synthesis

Physical method

Chemical method

Biological method

Ultrasonication, irradiation, laser ablation, microwave, electrochemical

Chemical reduction, sol gel method, inert condensation method

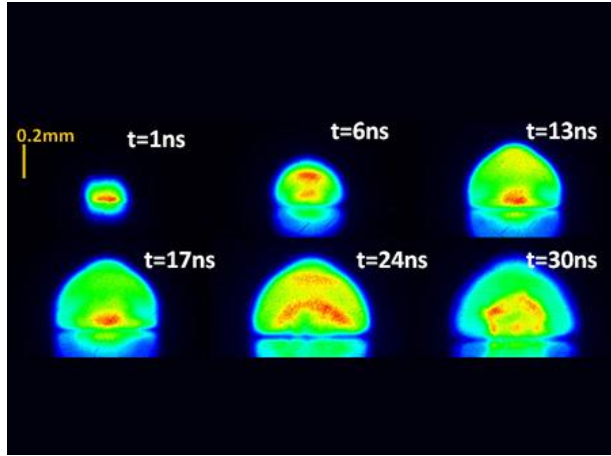
Microorganisms

Bacteria, fungi, algae, Yeast, Actinomycetes

Plants

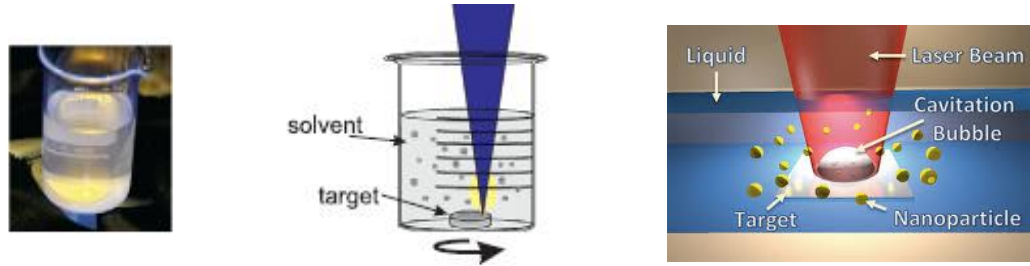
Gymnosperms  
To  
Angiosperms

# Laser Ablation and NP Formation



<http://appliedspectra.com/>

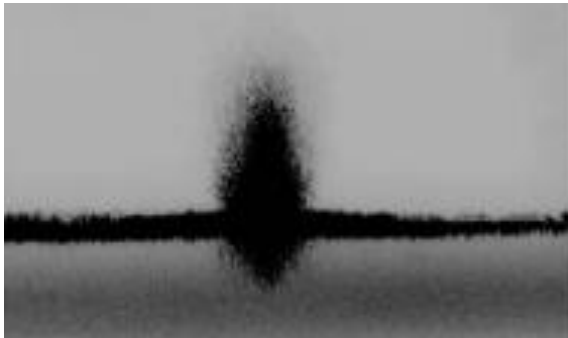
- Ablation threshold fluence
- Target material is heated and ejected
- Nanoparticles (NPs): in vacuum, in a background gas **or a liquid (colloidal nanoparticles)**



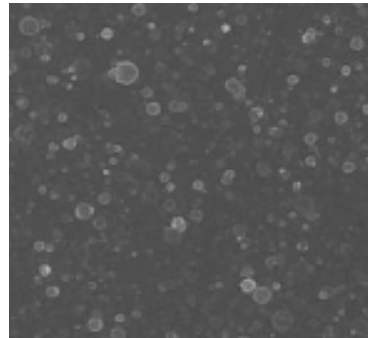
D. Amans et al. ILM, Lyon

Doi: 10.1007/978-3-030-63647-0\_30

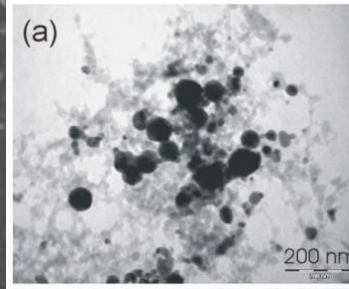
## Experimental evidences of nanoparticle formation by LA



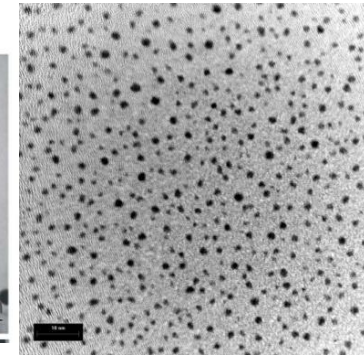
Heiroth et al. JAP 2009



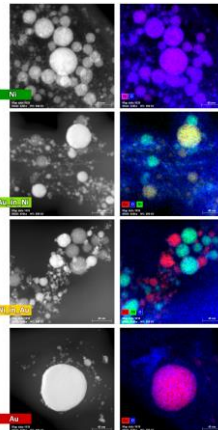
Deposited nanoparticles,  
courtesy of Garrelie et al.



Colloidal nanoparticles  
Barcikowski et al. APL 2007



TEM images  
Kabashin et al.



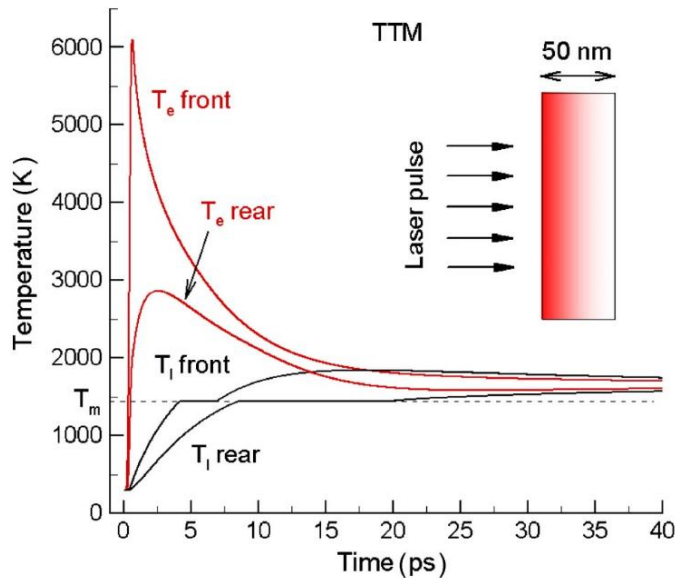
Z. Swaitkowska  
et al 4

# Main Questions Concerning Laser-based NP Formation

- What are the mechanisms of their formation?
- What roles do laser parameters play?
- What if we change target material?
- The role of ambient environment?
- Are there any control possibilities?
- Can more complicated nano-hybrids or nano-composites be directly fabricated by laser?
- For what specific applications these particles are most promising?
- How to predict/optimize the required nanoparticle's shape and morphology?
- If we can predict, how to fabricate them?



# Ultra-short Laser Interactions



## 1. Thermal (TTM) models

$$C_e \frac{\partial T_e}{\partial t} = \frac{\partial}{\partial z} \left( k_e \frac{\partial T_e}{\partial z} \right) - \gamma (T_e - T_i) + Q_{abs}$$

$$C_i \frac{\partial T_i}{\partial t} = \frac{\partial}{\partial z} \left( k_i \frac{\partial T_i}{\partial z} \right) + \gamma (T_e - T_i)$$

⇒ **Melting without ablation**

⇒ **Many assumptions**

⇒ **No motion**

⇒ **Hard to describe phase changes**

⇒ **Have to know many coefficients**

## 2. Molecular dynamics approach (MD or TTM-MD)

⇒ **melting, ablation**

⇒ **interaction potential is often assumed to be constant**

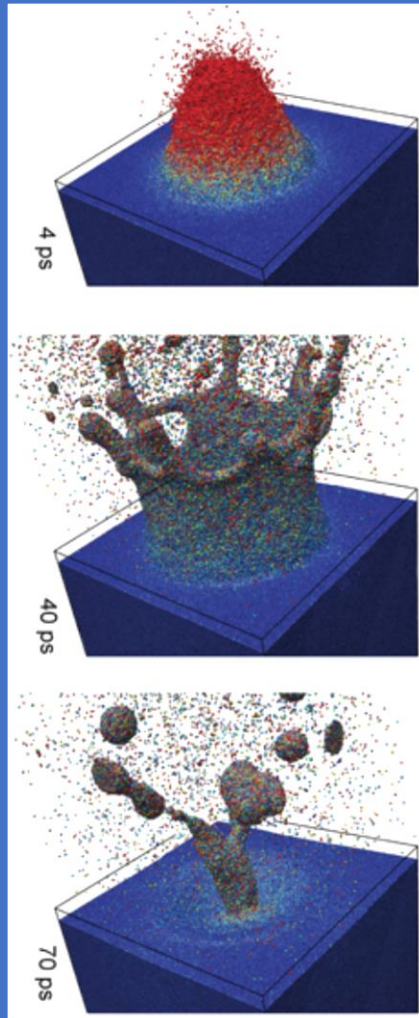
## 3. Hydrodynamics (1T, 2T, one fluid, two fluids, etc.)

⇒ **Need all transport coefficients**

⇒ **Need equation of state (EOS)**

⇒ **Need additional sub-models for ionisation**

# TTM-MD for Femtosecond Laser Ablation



InSIDE • Vol. 10 No. 1 • 2012

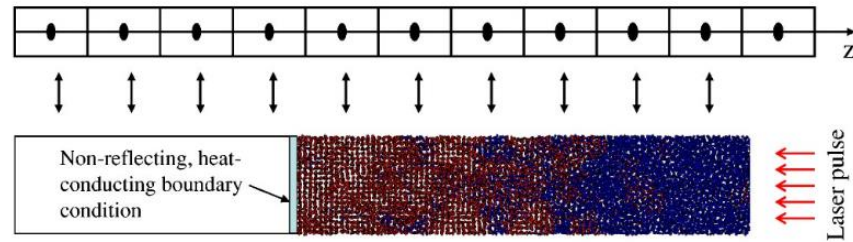
## Two-temperature model (TTM)

$$C_e(T_e) \frac{\partial T_e}{\partial t} = \nabla [K_e(T_e) \nabla T_e] - G(T_e - T_l) + S(z, t),$$

$$C_l(T_l) \frac{\partial T_l}{\partial t} = \nabla [K_l(T_l) \nabla T_l] + G(T_e - T_l),$$

Kaganov et al. Sov. Phys. JETP 4, 173 (1957)

## TTM-MD model



$$C_e(T_e) \frac{\partial T_e}{\partial t} = \frac{\partial}{\partial z} \left( K_e(T_e) \frac{\partial T_e}{\partial z} \right) - G(T_e - T_l) + S(z, t), \quad \text{TTM}$$

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i + \xi m_i \mathbf{v}_i^T, \quad \text{MD}$$

Ivanov & Zhigilei, PRB (2003)

$$\xi = \frac{1}{n} \sum_{k=1}^n G V_N (T_e^k - T_l) \bigg/ \sum_i m_i (\mathbf{v}_i^T)^2$$

# Ultra-short Laser Interactions

## CFD or MD?

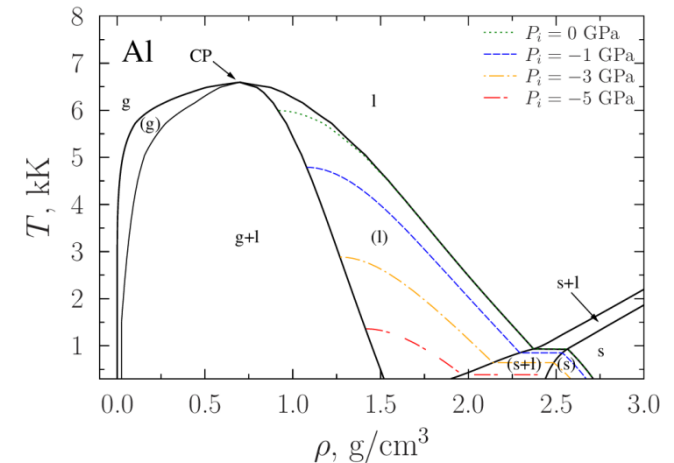
$$\frac{\partial(1/\rho)}{\partial t} - \frac{\partial u}{\partial m} = 0$$

$$\frac{\partial u}{\partial t} + \frac{\partial(P_{\text{ion}} + P_{\text{el}})}{\partial m} = 0$$

$$\frac{\partial e_{\text{ion}}}{\partial t} + P_{\text{ion}} \frac{\partial u}{\partial m} = \gamma_{ei}(T_{\text{el}} - T_{\text{io}})/\rho$$

$$\frac{\partial e_{\text{el}}}{\partial t} + P_{\text{el}} \frac{\partial u}{\partial m} = \frac{\partial}{\partial m} \left( \rho \kappa_{\text{el}} \frac{\partial T_{\text{el}}}{\partial m} \right) - \gamma_{ei}(T_{\text{el}} - T_{\text{ion}})/\rho + Q_L/\rho$$

EOS



$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i + \xi_i m_i \mathbf{v}_i^T + \mathbf{F}_i^{\text{el}} \quad \text{LAMMPS}$$

$$\frac{\partial(\rho e_{\text{el}})}{\partial t} + \frac{\partial(\rho e_{\text{el}} u)}{\partial z} + P_{\text{el}} \frac{\partial u}{\partial z} = \frac{\partial}{\partial z} \left( \kappa_{\text{el}} \frac{\partial T_{\text{el}}}{\partial z} \right) - \gamma_{ei}(T_{\text{el}} - T_{\text{ion}}) + Q_L(t, z)$$

Embedded atom "EAM"

$$E_i = F_{\alpha} \left( \sum_{j \neq i} \rho_{\beta}(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$$

Zhakhovskii *et al.* Appl. Surf. Sci. 255 (2009)

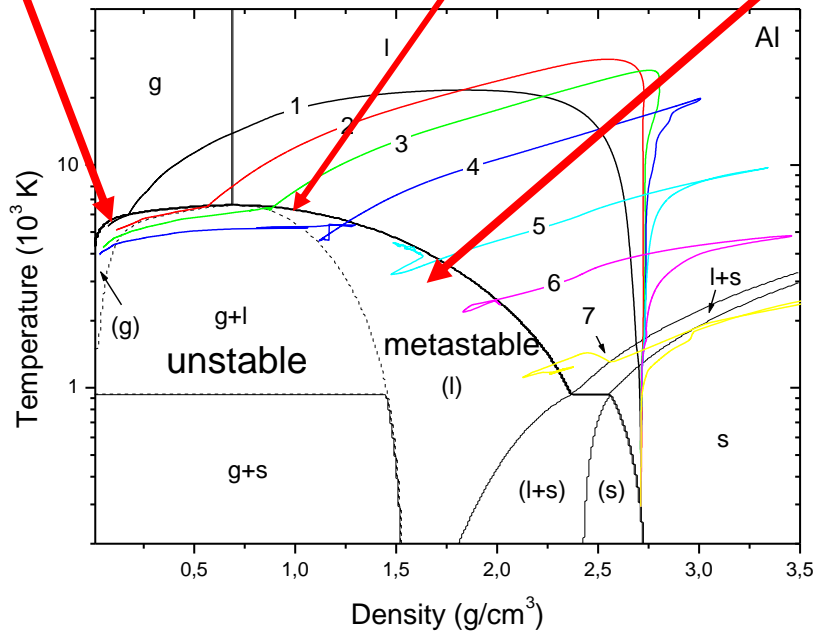
# Thermodynamic Analysis of Laser Ablation

3-Nucleation and condensation

1-Phase explosion

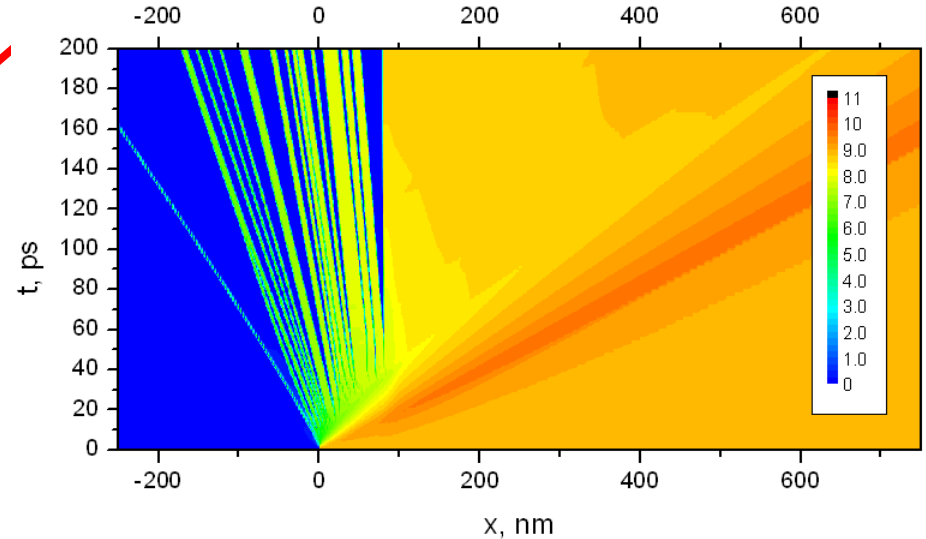
2- Fragmentation

$$0.9T_c < T < T_c$$

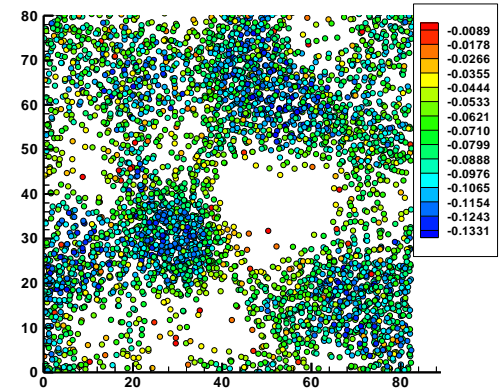


$$\tau_L = 100 \text{ fs}, \lambda = 800 \text{ nm}, F = 5.0 \text{ J/cm}^2$$

**Explosive boiling and fragmentation of metastable liquid lead to the ejection of clusters and chunks**



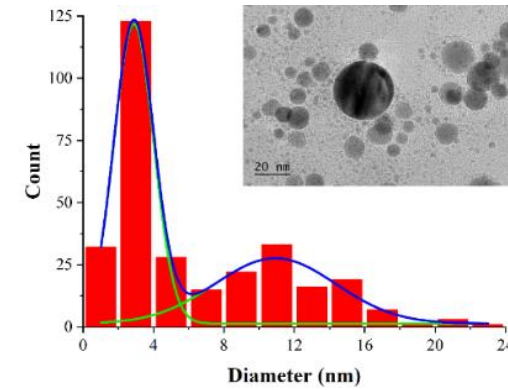
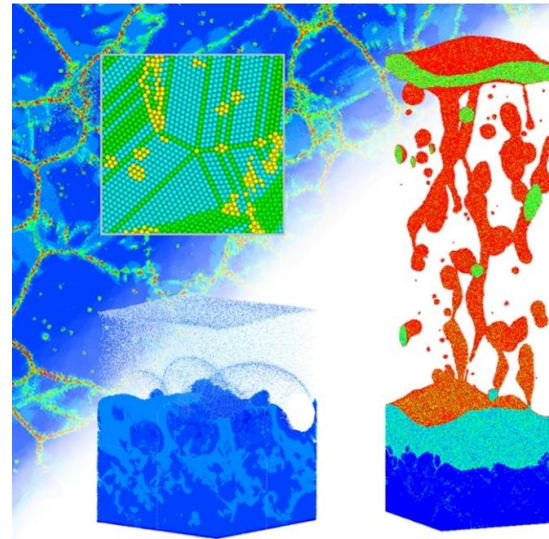
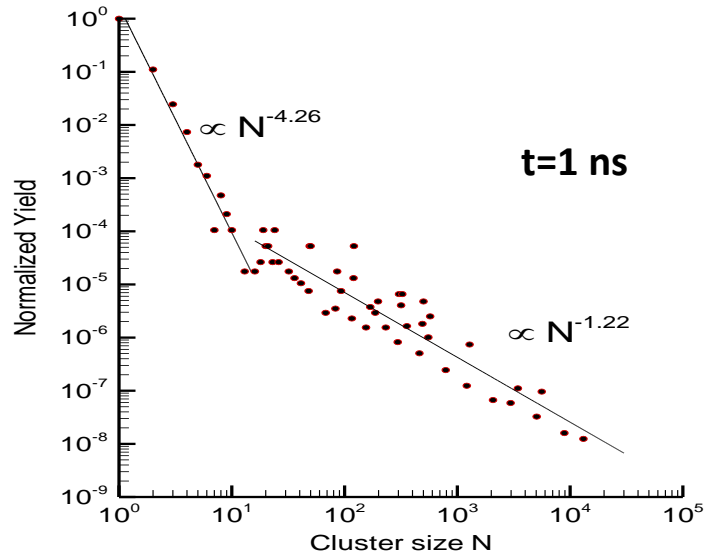
*M.E. Povarnitsyn, T. E. Itina et al. Phys. Rev. B, 75, 235414 (2007)*



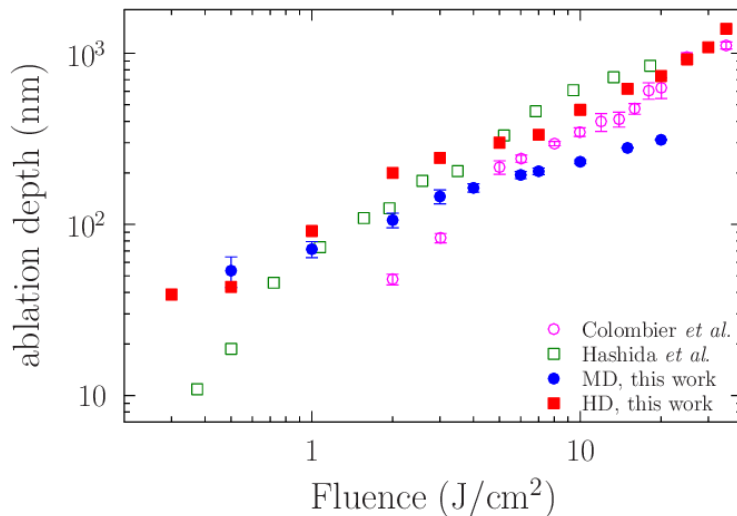
*T.E. Itina, Chem. Phys. Lett. (2008)*

# Molecular Dynamics Simulations

Allow to get nanoparticle size distributions and describe non-equilibrium processes



$\tau = 15$  ps,  $F \sim 2$  Fth,  $40 \times 10$  nm,  $t = 1$  ns



*L.V. Zhigilei et al.*

(Virginia State University, USA)

*A. Kabashin et al.*

LP3, Marseille, France

Practically all the molten material is ablated

$$Labl \sim Lo \ln(Fabs/F_0), E > Eb$$

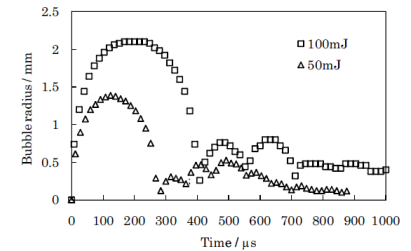
See: *M.E. Povarnitsyn, T. E. Itina et al., PRB 2007*

# Laser Ablation in Liquids

- confinement, different ablation threshold and yield
- shock wave formation
- bubble formation and oscillations
- “primary” nanoparticles are ejected
- “Secondary” particles are formed later by coagulation, coalescence/aggregation (sintering)
- fragmentation and stabilisation

## Confinement by liquid, oscillating bubbles

$$R_n(t) = \left\{ R_{na}^3 + \frac{R_{nb}^3 - R_{na}^3}{2\tau} \left[ t - \frac{\tau}{\pi} \sin\left(\frac{\pi}{\tau} t\right) \right] \right\}^{1/3}$$



See: A. Vogel et al., J. Acoust. Soc. Am. 100(1), 1996

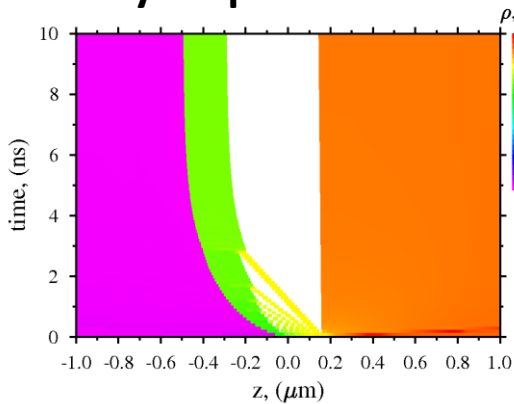
**Modeling approaches:**  
**Hydrodynamic modeling (CFD)**  
**Molecular Dynamics (MD)**

- *2T semi-empirical equations of state (for metal, gold here)*
- *EOS for water*

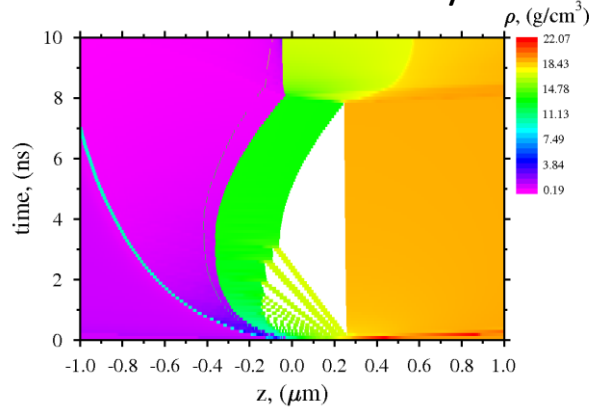
# Single fs Laser Pulse in Liquids: TTM-HD

Density maps

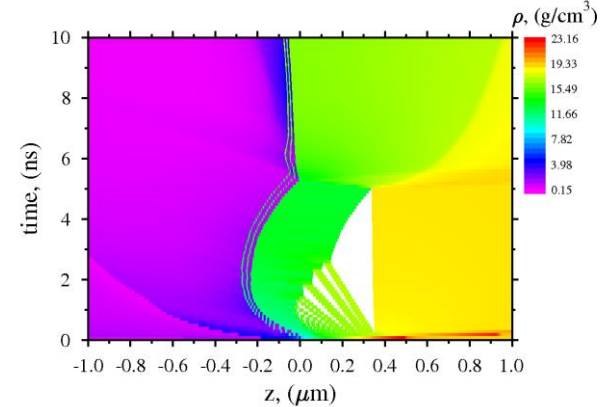
$3 \times 10^{13} \text{ W/cm}^2$



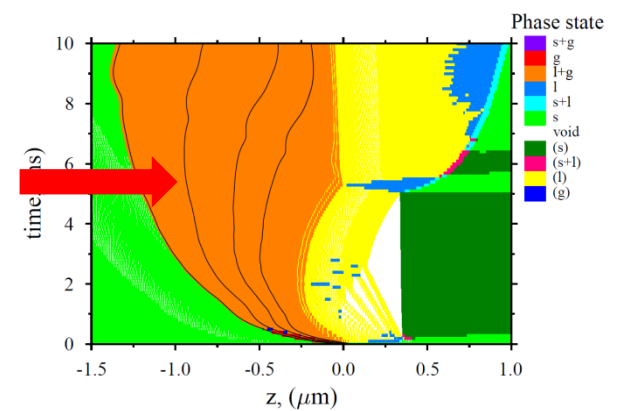
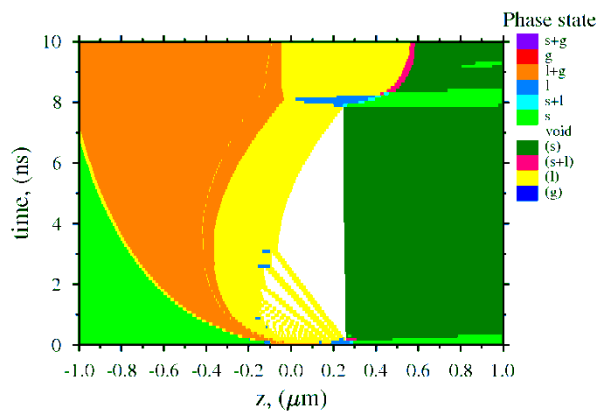
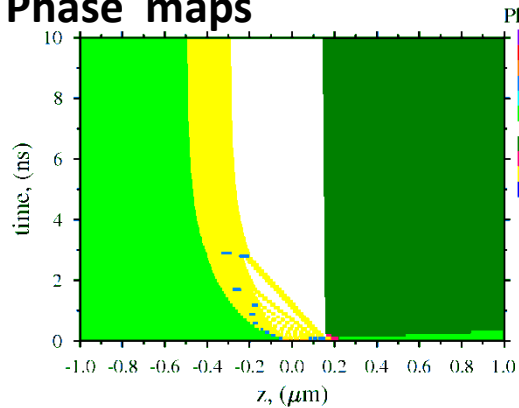
$4 \times 10^{13} \text{ W/cm}^2$



$5 \times 10^{13} \text{ W/cm}^2$



Phase maps



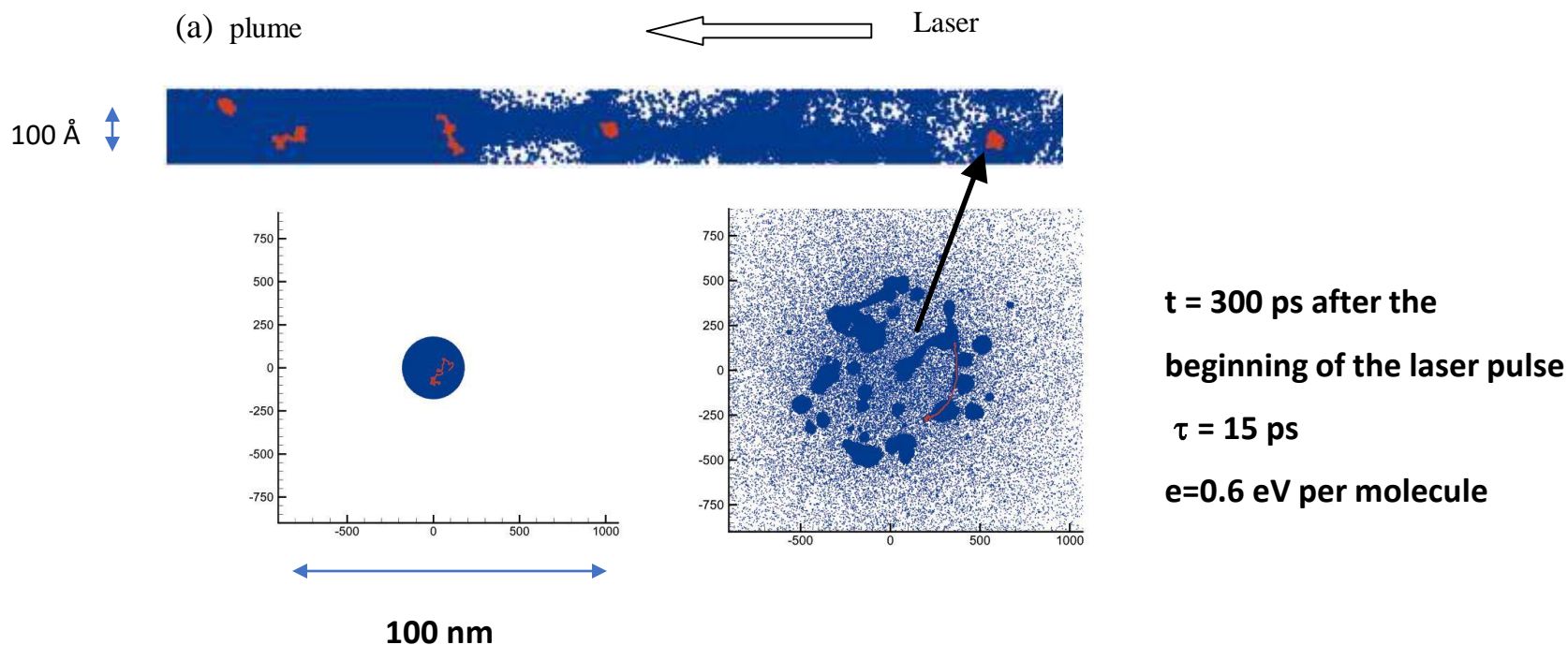
Near ablation threshold, ejected droplets stick together under the pressure

Povarnitsyn, Itina et al. PCCP 9 (2013)

NPs are formed in the metastable and in the unstable liquid phases, later additional condensation and growth also take place.

# Laser Interactions with Nanoparticles

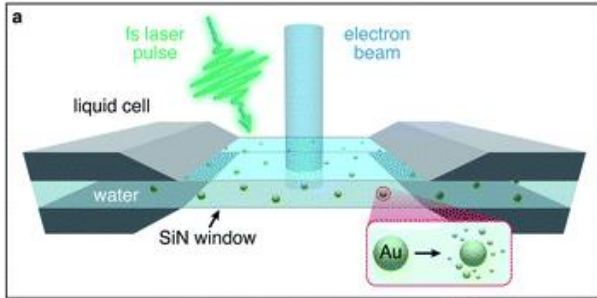
Molecular Dynamics (MD) simulations are particularly interesting for phase transitions and decomposition of the ablated material upon the absorption of laser radiation, but also can be used for heating, melting, fragmentation or sintering of NPs



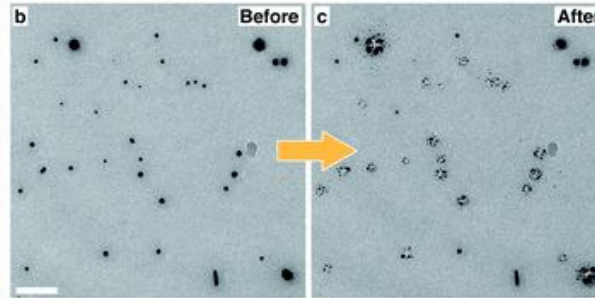
*T. E. Itina, L. V. Zhigilei, B. J. Garrison*  
*The Journal of Physical Chemistry B 106 (2), 303-310 (2002)*

# NP's Fragmentation: Experiments and MD Simulations

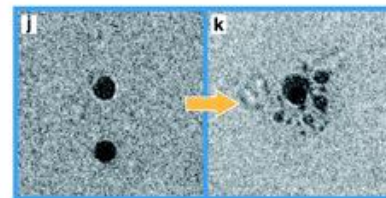
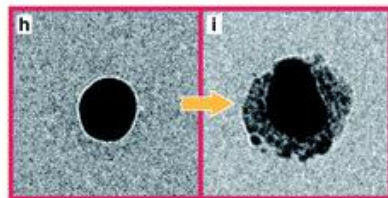
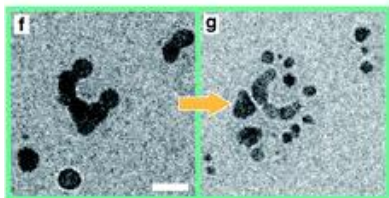
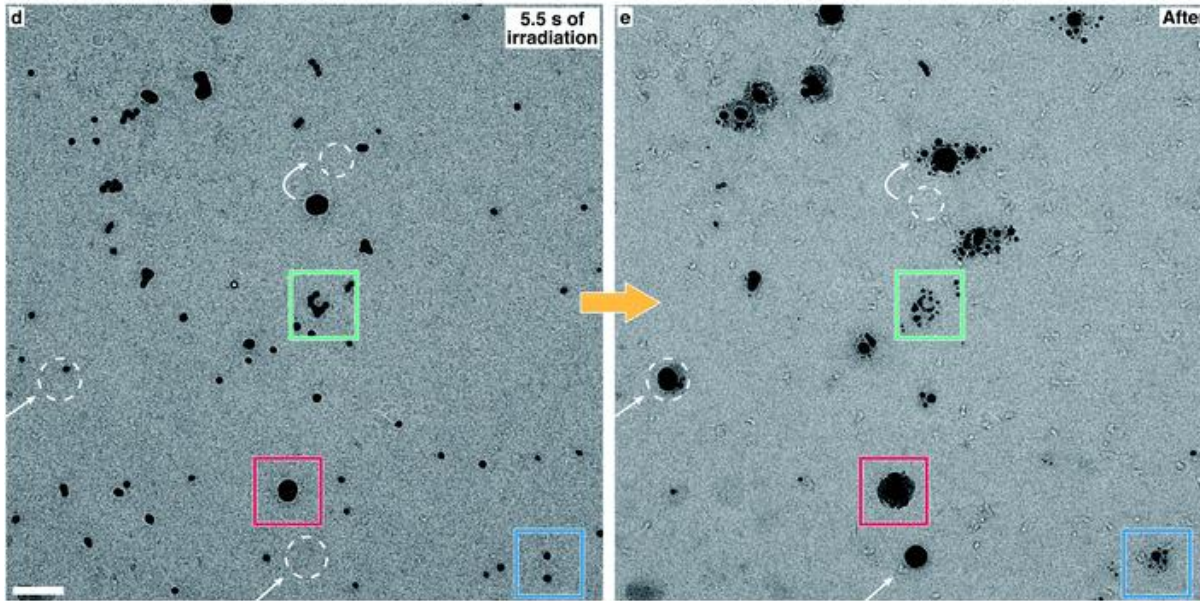
Experimental geometry



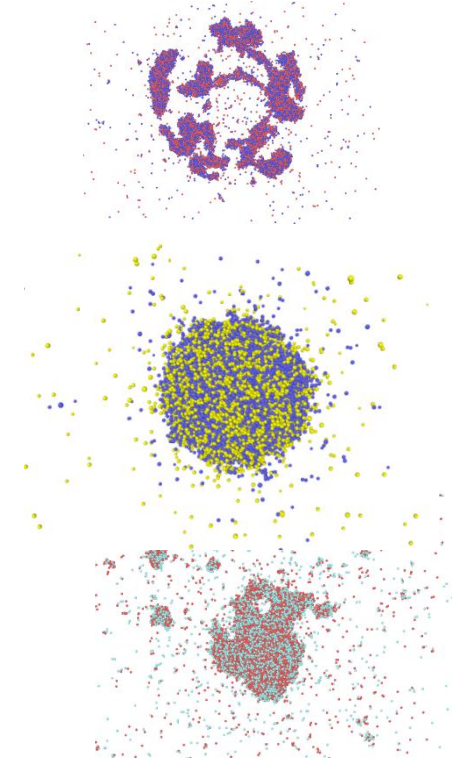
Femtosecond laser irradiation of gold nanoparticles



In situ observation of gold nanoparticle fragmentation under femtosecond laser irradiation

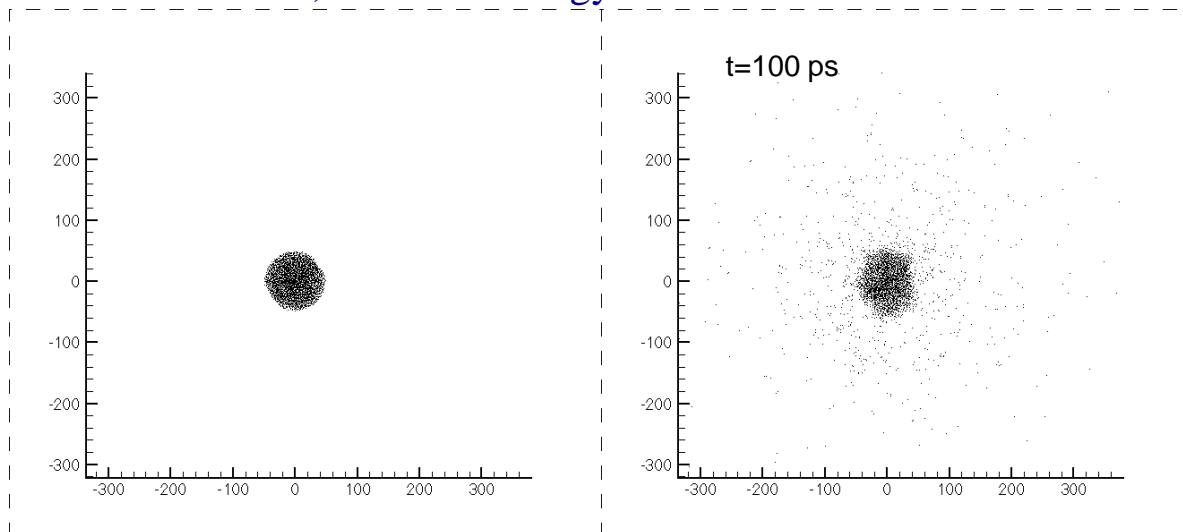


MD results for NPs of different materials, absorbed energy, and sizes



# Laser Interaction with Organic NPs: Early MD Simulations

$R=50 \text{ \AA}$ , absorbed energy  $e=0.6 \text{ eV/mol}$

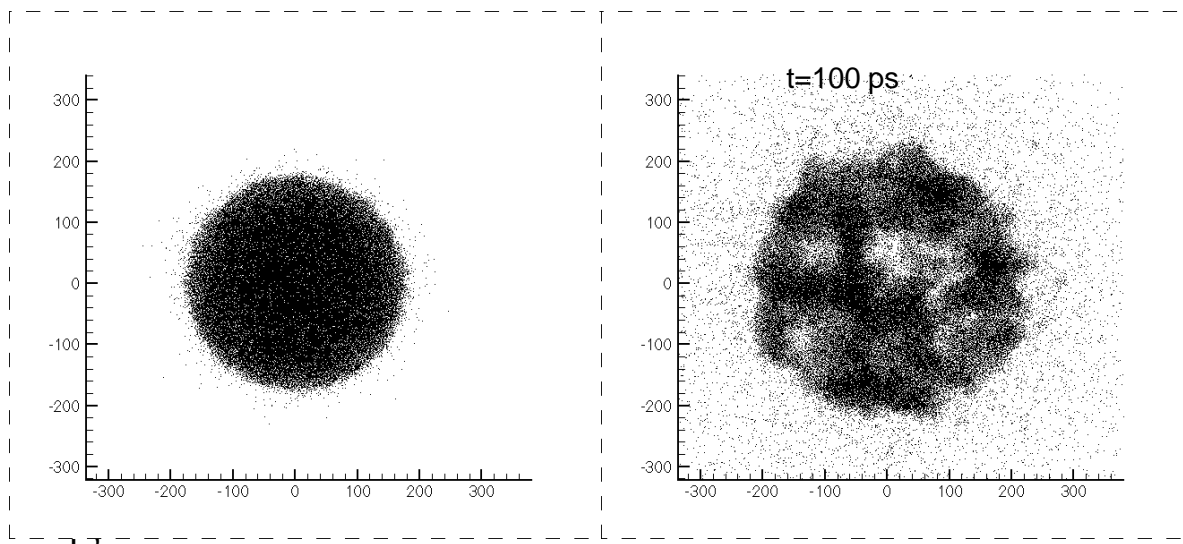


Smaller NPs

**Evaporation**

(can be also due to Coulomb Explosion for small clusters and fs laser)

$R=150 \text{ \AA}$ , absorbed energy  $e=0.6 \text{ eV/mol}$ .



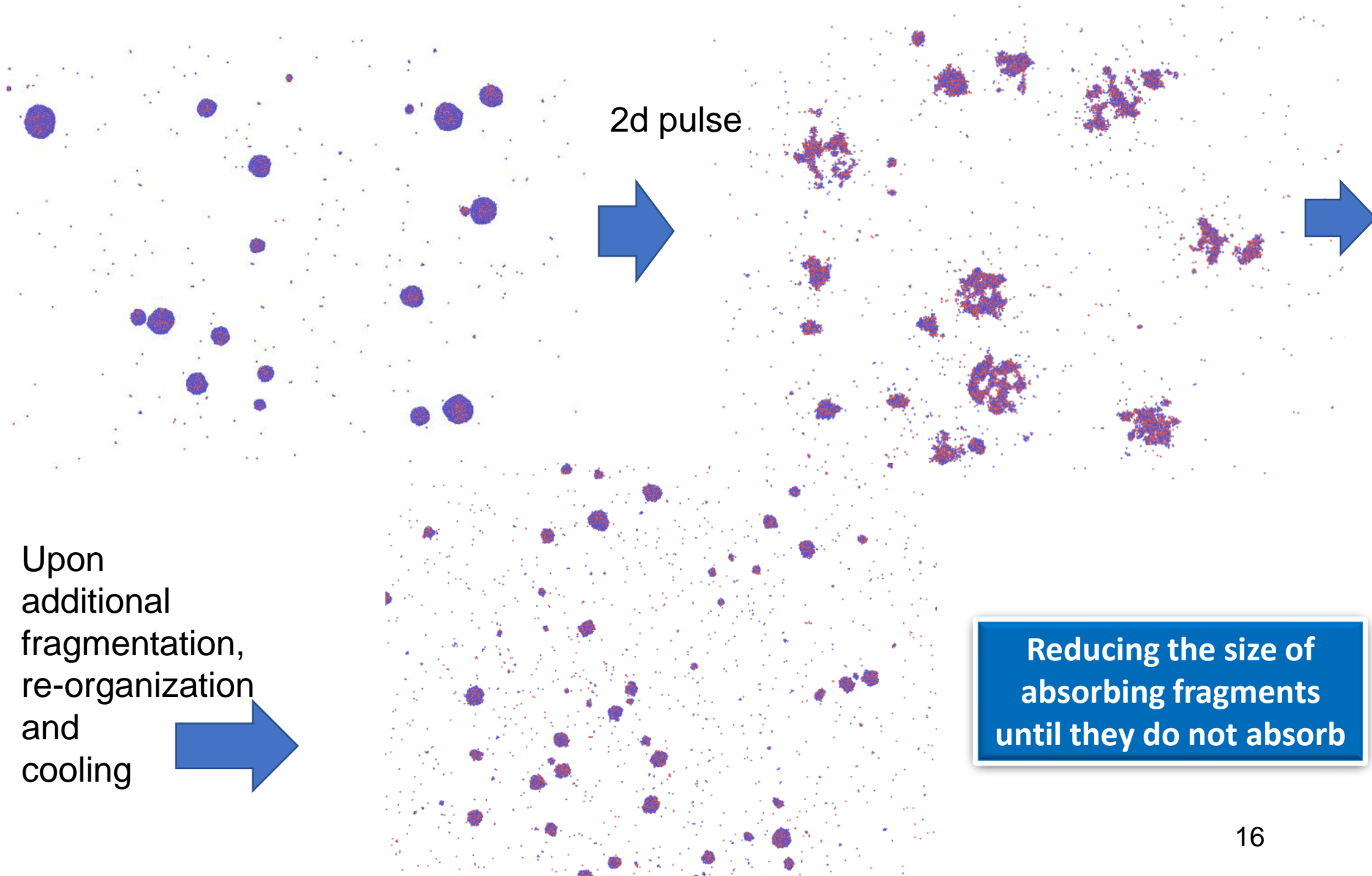
Larger NPs

**Fragmentation due to thermo-mechanical effects**

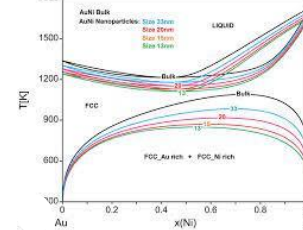
# Fragmentation When There Are Many Laser Pulses

AuCo, NP R = 40 u.c.

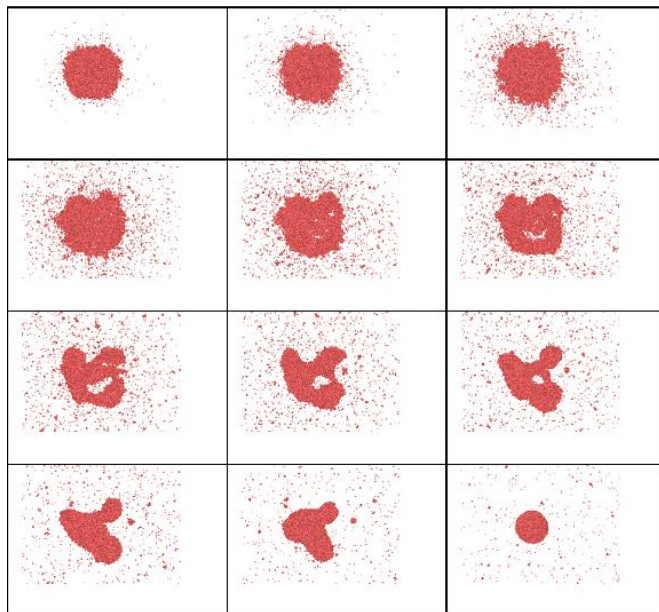
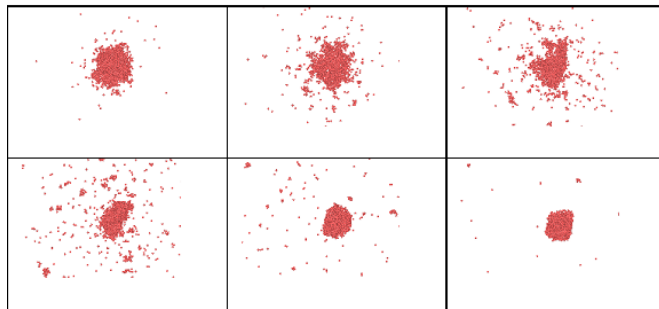
Multi-pulse effects: simulations re-start additional fragmentation



# MD Simulations for Au, Au-Ni and AuNi

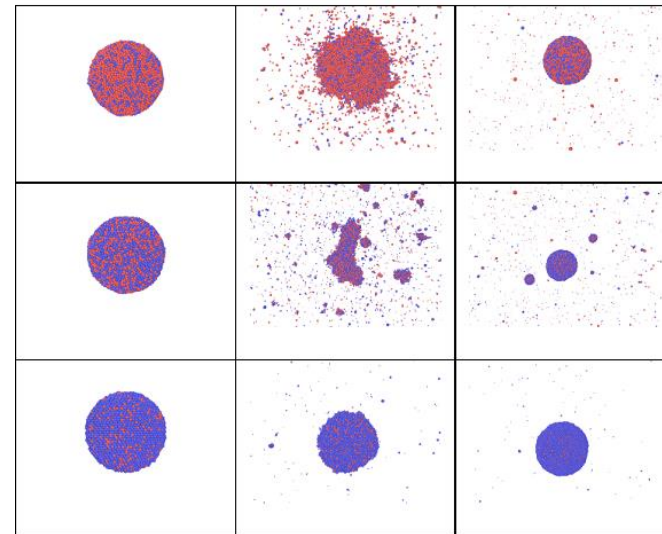


Fragmentation of a single Au NP



$T_{max} > T_c$

Ni-Au alloys

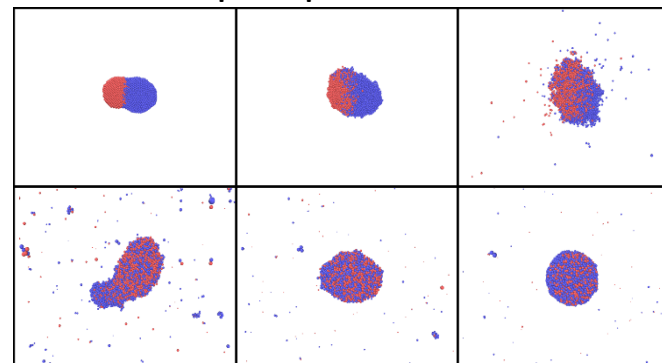


20% Ni

50% Ni

80% Ni

Janus NP upon pulsed laser irradiation

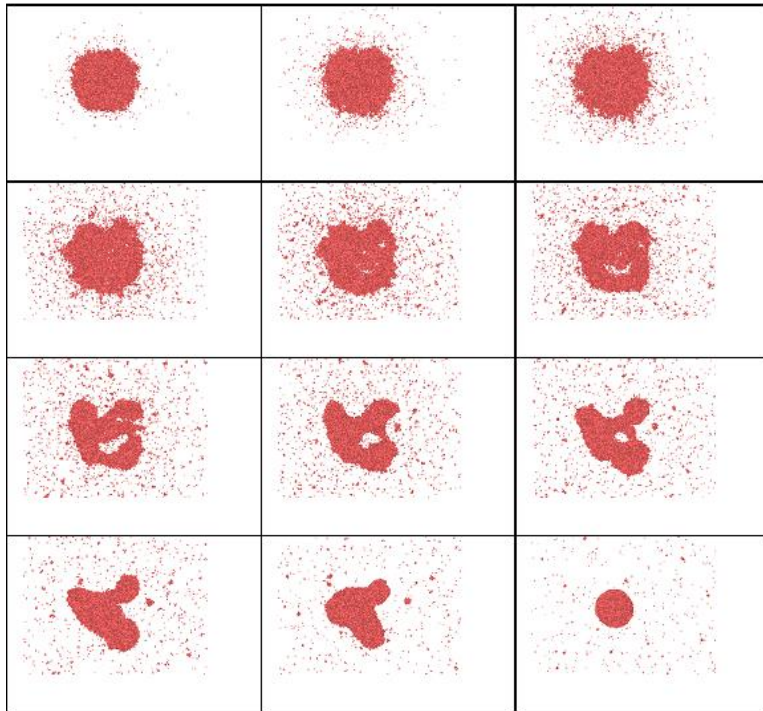


High  
 $T_{max}$   
above  
2600 K

# Laser Interaction with Metallic NPs

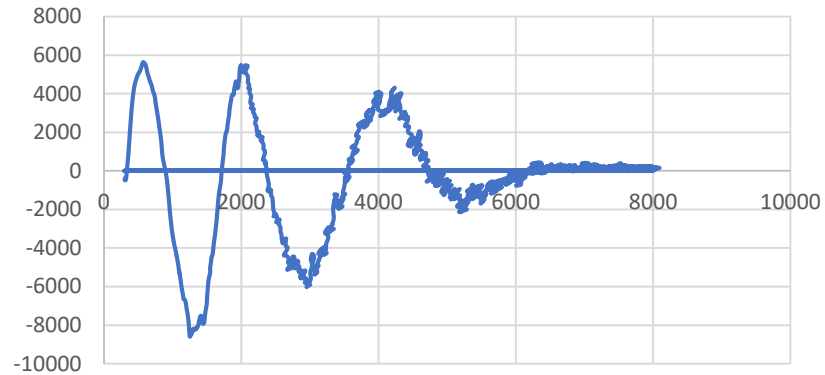
Vibrations and  
fluid instabilities

$T_{max} > T_c$

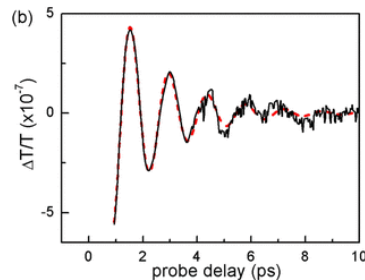
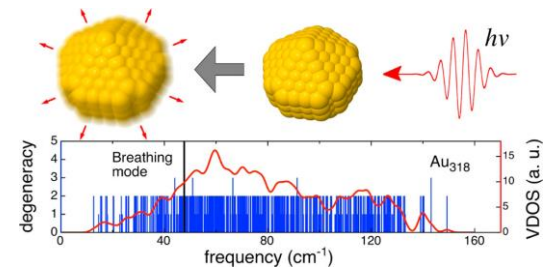
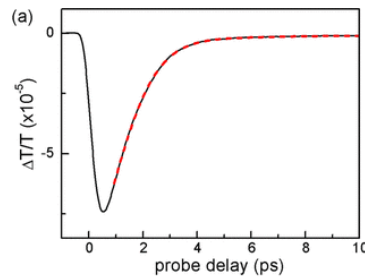


Au nanocluster with  $N=30845$  atoms and maximum temperature  $T_{max}=8000K$  obtained at time delays  $t=0.1, 5, 10, 20, 50, 100$  ps after the beginning of strong and short (20ps) heating

## Pressure vs Temperature

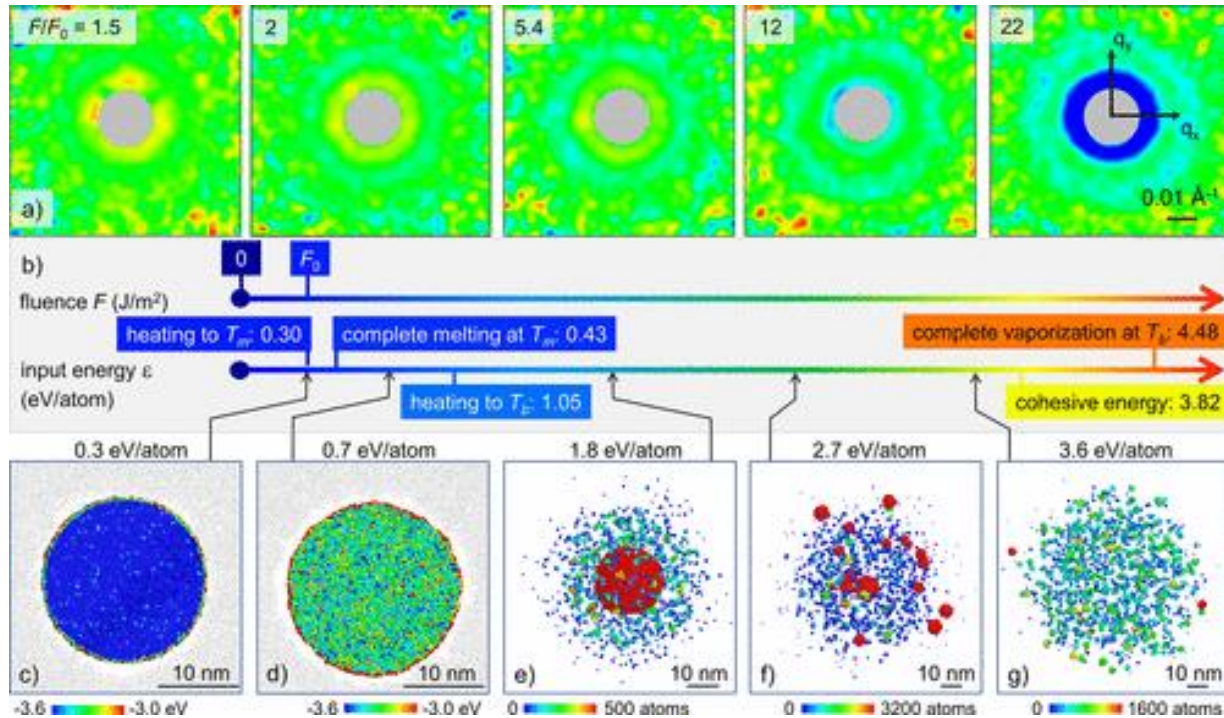


T. E. Itina, RCS Nanoscale Advances 6, 5451 (2024)



[\*H. E. Saucedo et al. J. Phys. Chem. C, 116 \(47\), 2012\*](#)

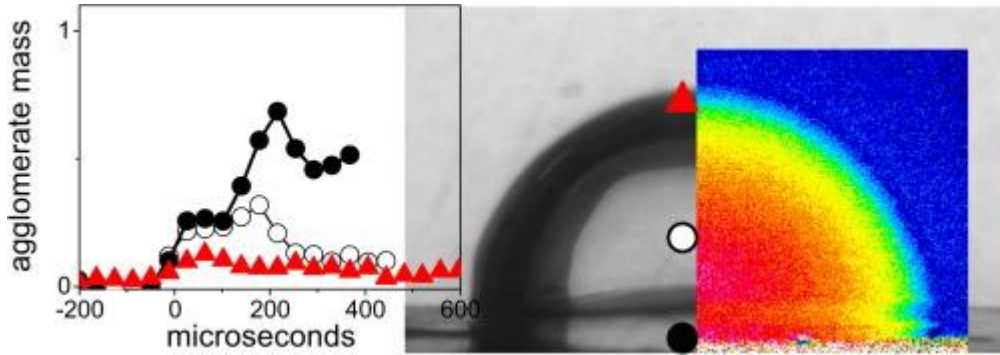
# Fs Laser Interactions with Metallic NPs in Liquids



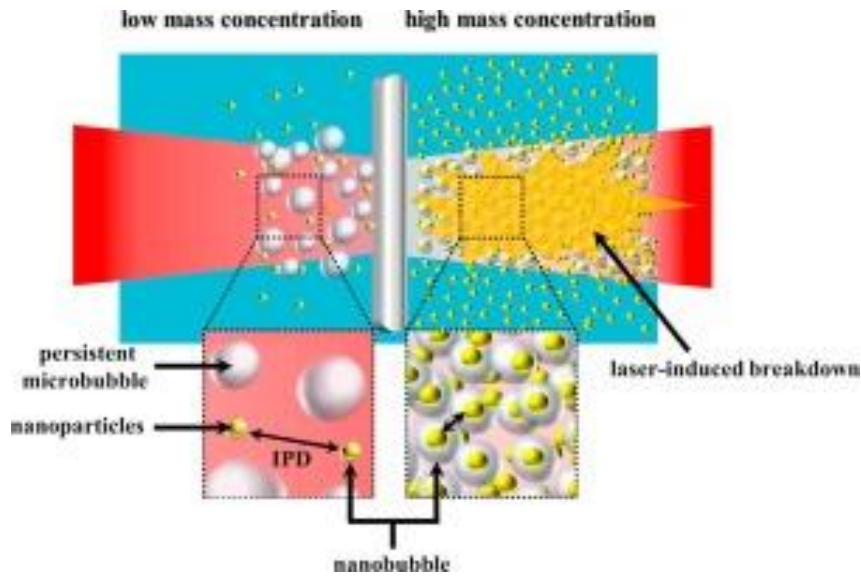
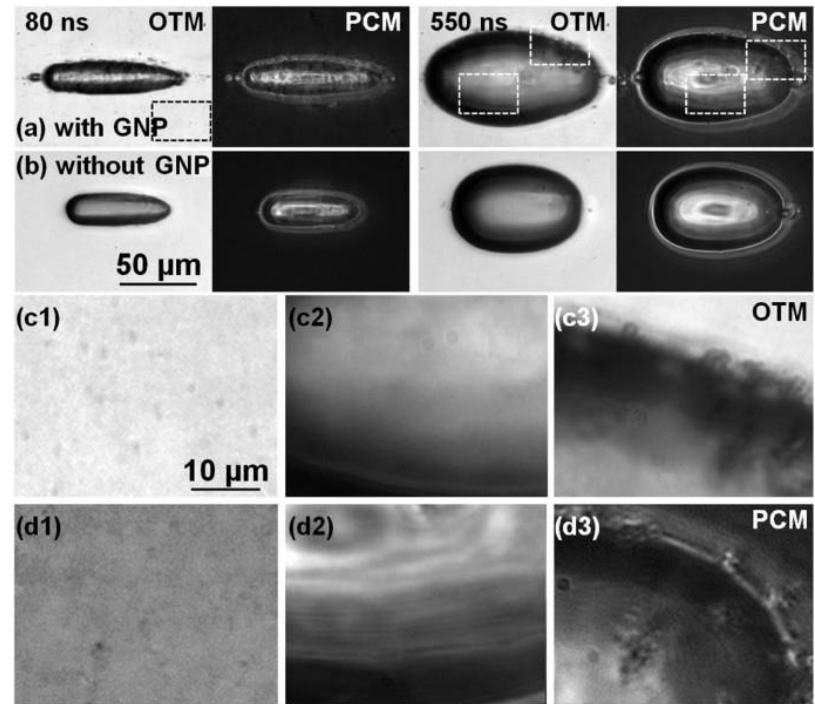
- Heating Au to  $T_m$ ,  $\epsilon_0 = 0.3$  eV/atom;
- complete melting of Au at  $T_m$ ,  $\epsilon = 1.43$ ,  $\epsilon_0 = 0.43$  eV/atom;
- heating Au to the boiling temperature of  $T_b = 3131$  K,  $\epsilon = 3.5$ ,  $\epsilon_0 = 1.05$  eV/atom;
- completely vaporizing Au at  $T_b$ ,  $\epsilon = 14.9$ ,  $\epsilon_0 = 4.48$  eV/atom.

[A. Plech et. al, ACS Nano Vol 18/Issue 15, 2024](#)

# In Liquids: Bubbles and Nanoparticles



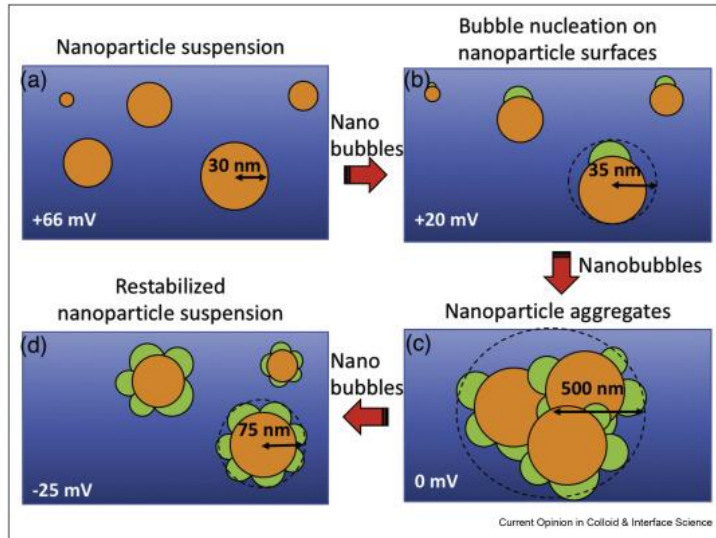
[S. Reich et al. Journal of Colloid and Interface Science Volume 489, 1 March 2017, Pages 106-113](#)



[M.-R. Kalus et al. Applied Surface Science Volume 465, 28 January 2019, Pages 1096-1102](#)

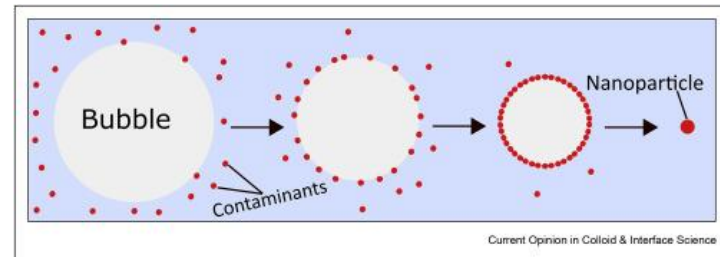
[M. K. Bhuyan et al. Scientific Reports 8, 9665 \(2018\)](#)

# In Liquids: Bubbles And Nanoparticles



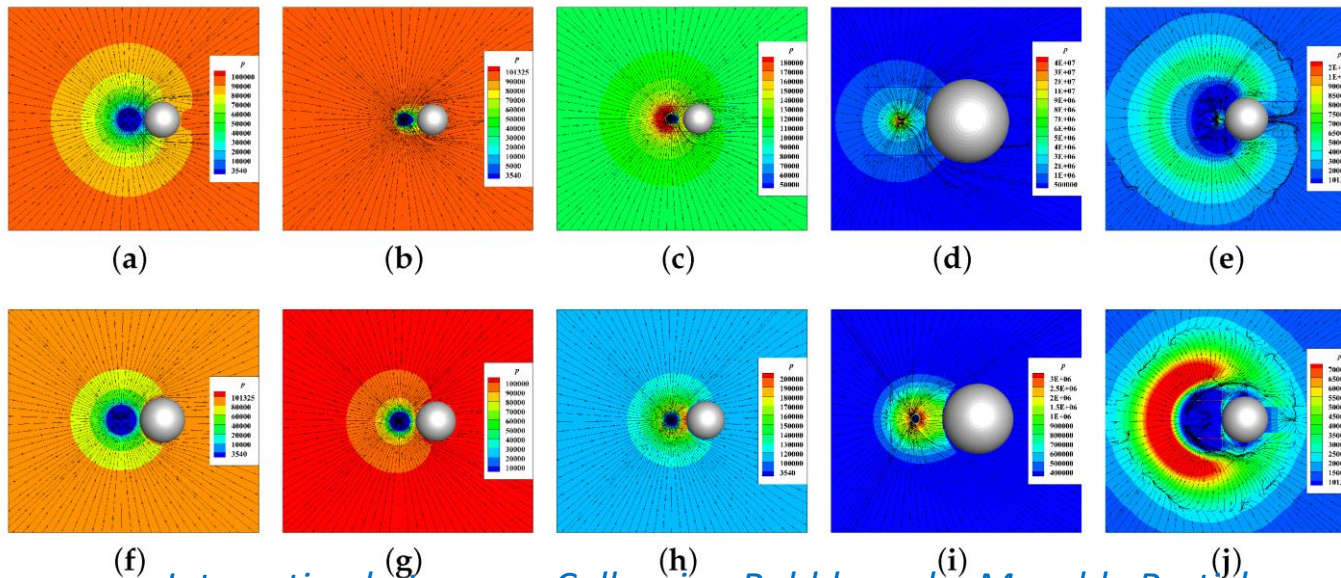
M. Alheshibri et al.

## Interaction between bulk nanobubbles and positively charged nanoparticles



*Current Opinion in Colloid & Interface Science*

*Volume 55, October 2021, 101470*



*Interaction between a Collapsing Bubble and a Movable Particle,*

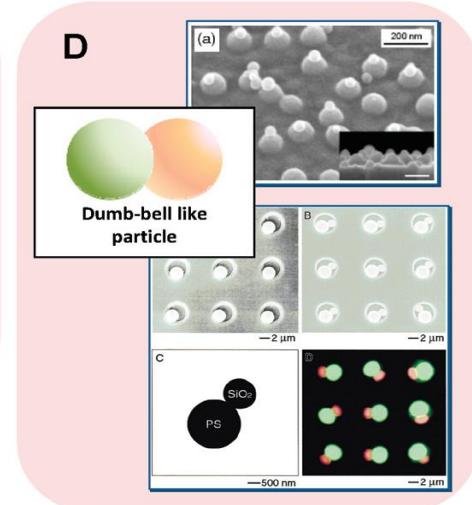
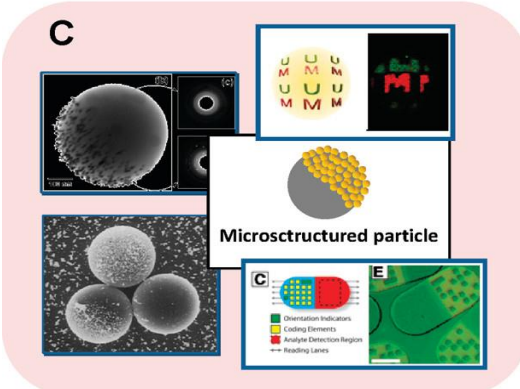
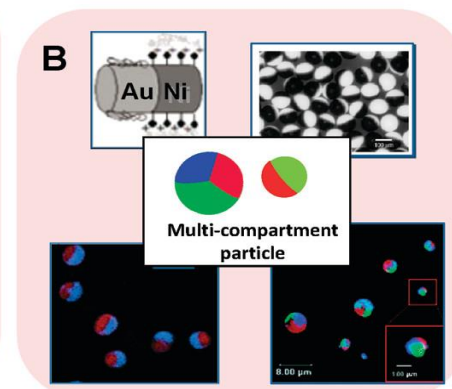
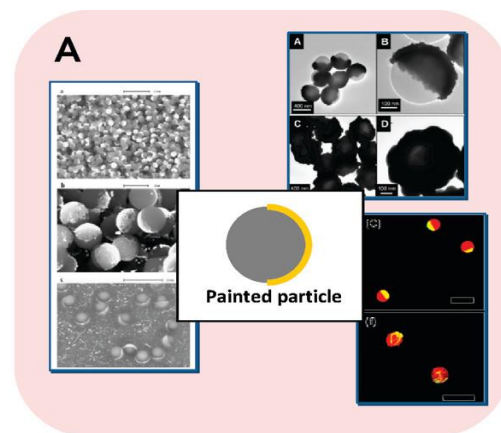
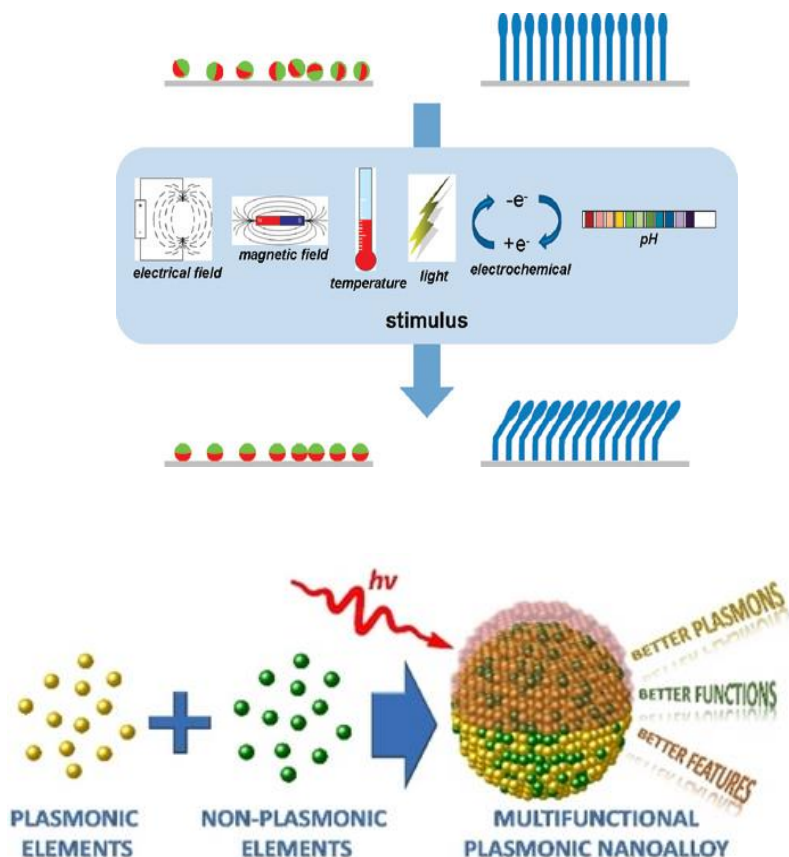
*X. Zheng et al. Water 2020, 12(12), 3331*

OpenFOAM  
CFD  
Simulations

Force balance  
model

# PLA for Synthesis of Smart Nanomaterials

Materials that respond to a stimulus or their environment to produce a dynamic and reversible change

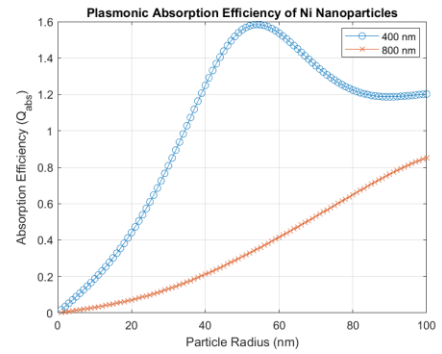
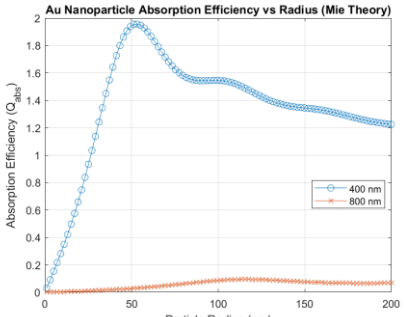


*V. Coviello et al*  
*ChemPhysChem* 2022  
*V. Amendola et al., Italy*

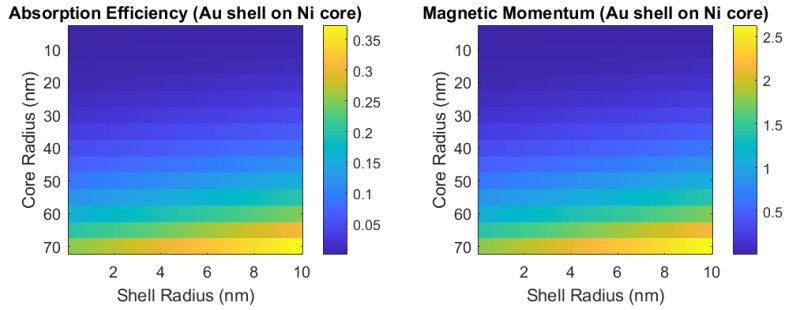
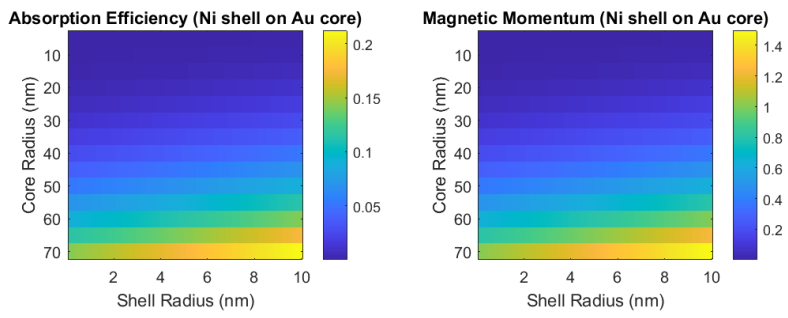
Laser give many possibilities: sintering, alloying, fragmentation, etc.

# Predictions of NP's Properties for Applications

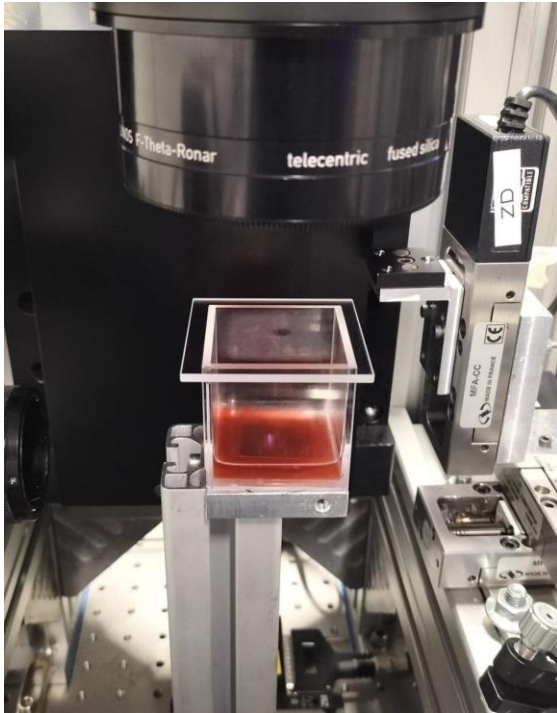
Configuration	Plasmonic Properties	Magnetic Properties	Optimal Size Range	Applications
Core-Shell Au-Ni	Strong plasmonic resonance at 520 nm (visible)	Moderate magnetic properties from Ni shell	20 nm Au core + 10 nm Ni shell	Photothermal therapy, magnetic targeting, drug delivery
Core-Shell Ag-Fe	Strong plasmonic resonance at 400-450 nm (visible)	Strong magnetic properties from Fe shell	20 nm Ag core + 10 nm Fe shell	Sensing, hyperthermia, MRI contrast agents
Au-Ni Nanorods	Tunable plasmonic resonance in NIR range	Moderate magnetic properties from Ni shell	30-40 nm length, 10-20 nm diameter	Optical sensing, NIR therapy, magnetic applications



Mie Theory Absorption and Magnetic Momentum for Ni-Au Core-Shell Nanoparticles



# Fabrication Methods: Fs Laser Co-Ablation



1030 nm

- Fluence: 10 J/cm<sup>2</sup>
- Frequency: 10 kHz
- Pulse duration: 450 fs
- Target placed 10 mm under liquid surface
- Volume of liquid: 6 ml
- Irradiation time: 30 min -3h

- „Au\_in\_Ni” stands for gold ablated in the presence of Ni NPs
- „Ni\_in\_Au” is for reversed configuration: nickel ablated in presence of Au NPs

## **Experiments:**

*Z. Switkowska, O. Polit, et al.*

*PAN Krakow, Poland*

*A. Pastukhov,*

*A. Kabashin et al.*

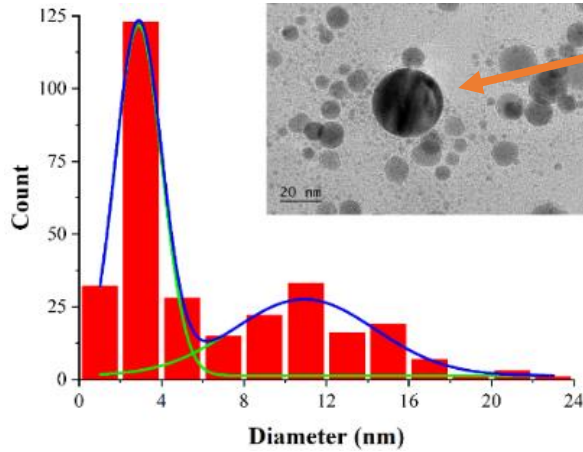
*LP3, Marseille, France*

**(PHC POLONIUM PROJECT)**



# Molecular Dynamics Simulations (MD) vs Experiments

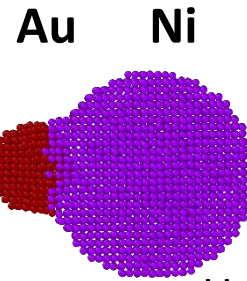
Au NP on Ni NP



Maximum temperature, K

Upon 1<sup>st</sup> heating and quenching

Upon 2<sup>st</sup> heating of 20 ps and cooling

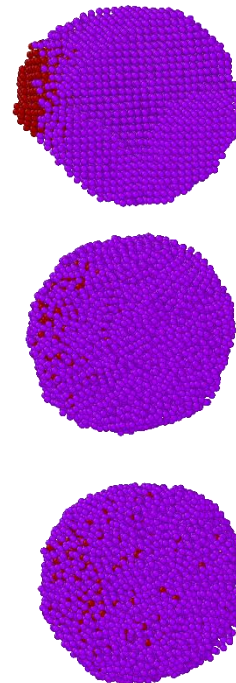
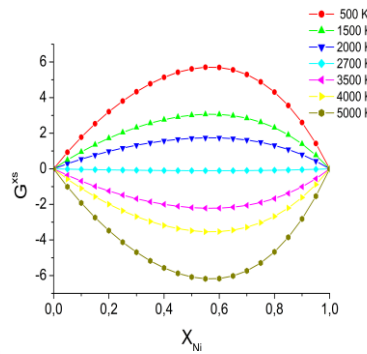
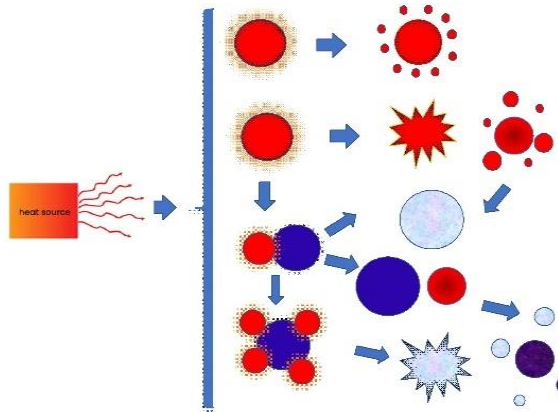


$T_{max}, K$

1200

2200

4200

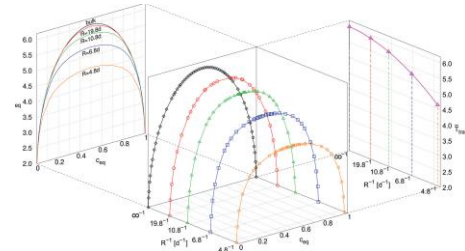
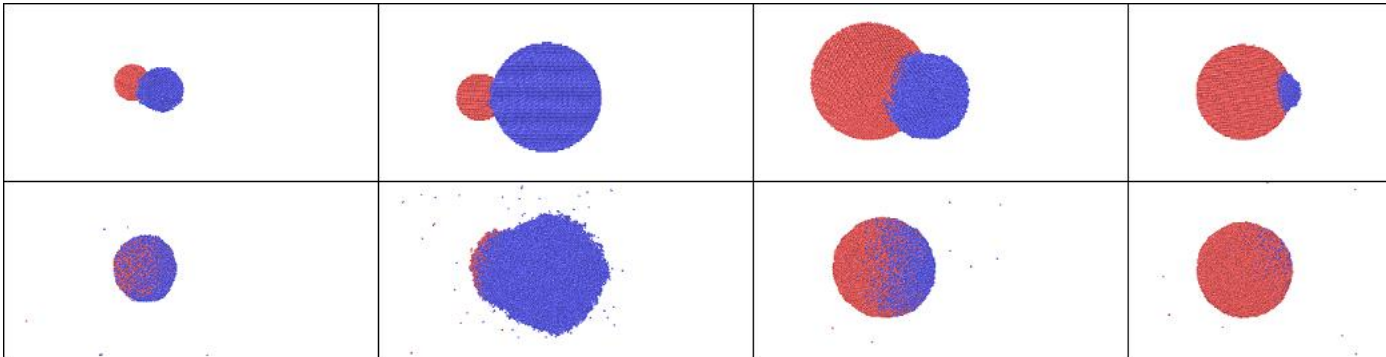


T. E. Itina, *Nanoscale Adv.*, 2024,  
6, 5451 DOI: 10.1039/D4NA00634H

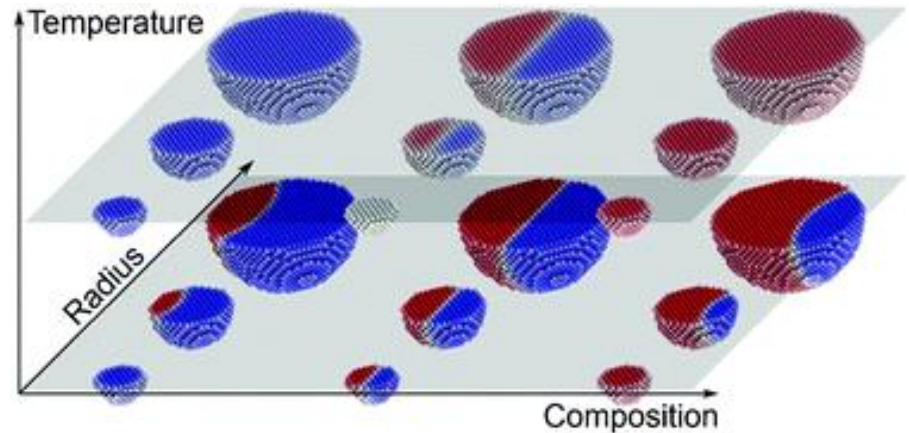
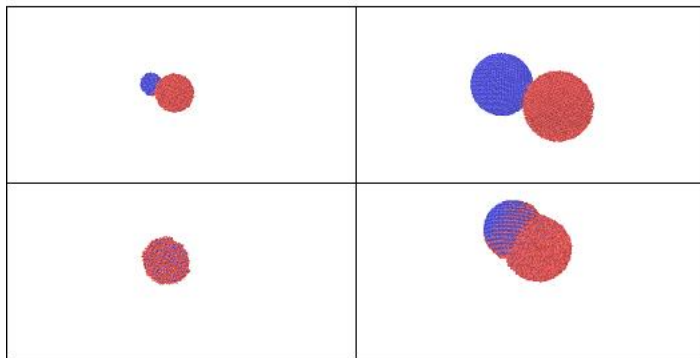
T.E. Itina et al *Lase* 2025

# Excess Gibbs Energy and Phase Diagrammes

Au and Ni Pulsed heating of Ni and Au NP, maximum  $T=5500\text{ K}$



Au and Pt  $T=\text{const}=1100\text{ K}$

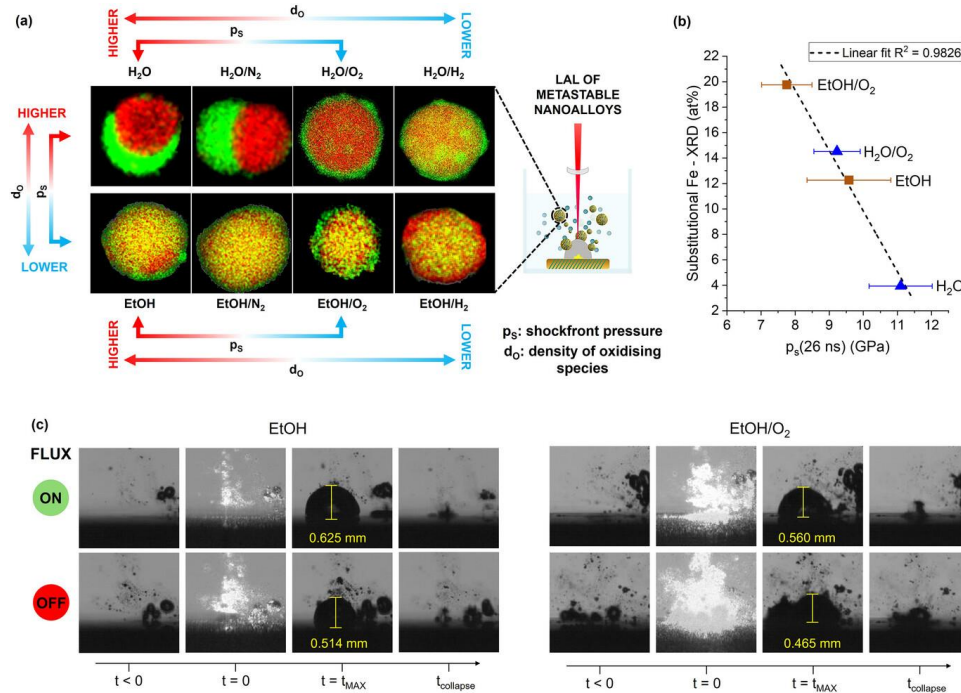


*A. Taranovskyy et al. Phys. Chem. Chem. Phys., 2021, 23, 6116-6127*

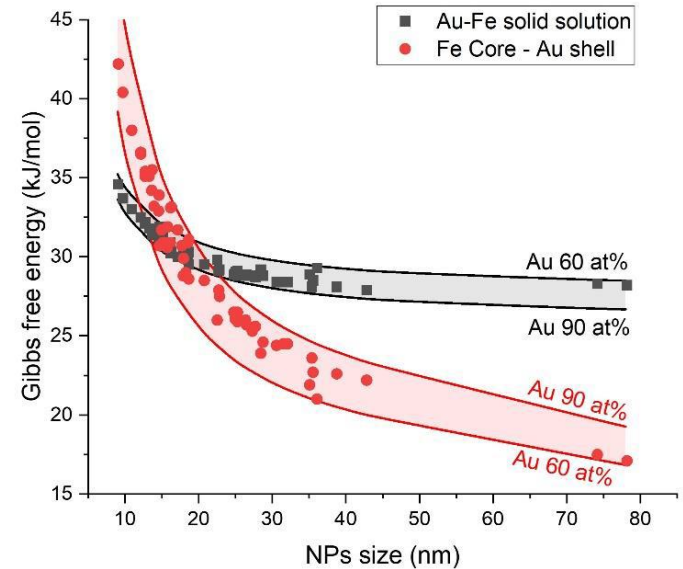
The results mostly rely on change in Gibbs energy, which depends on

- Temperature
- Composition
- Sizes

# Thermal Stability of Alloy, Janus or Core-Shell NPs



## Au and Fe NP



## Gibbs free energy for Alloy NPs ( $G_{SS}$ )

$$G_{SS} = X_{Au}G_{Au} + X_{Fe}G_{Fe} + \Delta G_{mix} + (2 \gamma_{SS} V_{AuFe}) / (D/2)$$

## Gibbs free energy for CS NPs ( $G_{CS}$ )

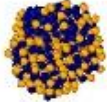
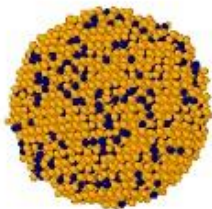
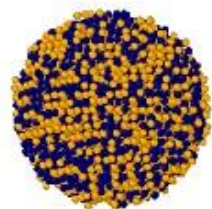
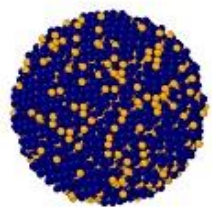
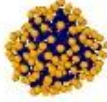
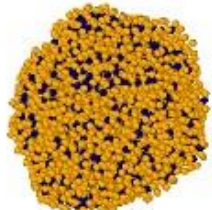
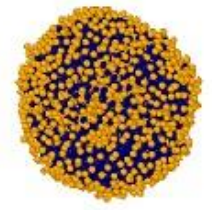
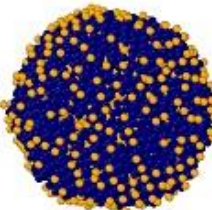

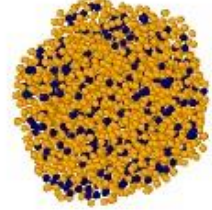
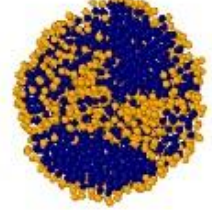
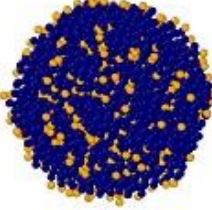
$$G_{CS} = X_{Au}G_{Au} + X_{Fe}G_{Fe} + \alpha_{Au} S_{Au} \gamma_{Au} + \alpha_{Fe} S_{Fe} \gamma_{Fe} + G_{int}$$

V. Coveillo et al. *Advanced Science*, 2025  
DOI 10.1002/advs.202416035

ARQUS project with:  
Group Prof. V. Amendola,  
Padova University, Italy

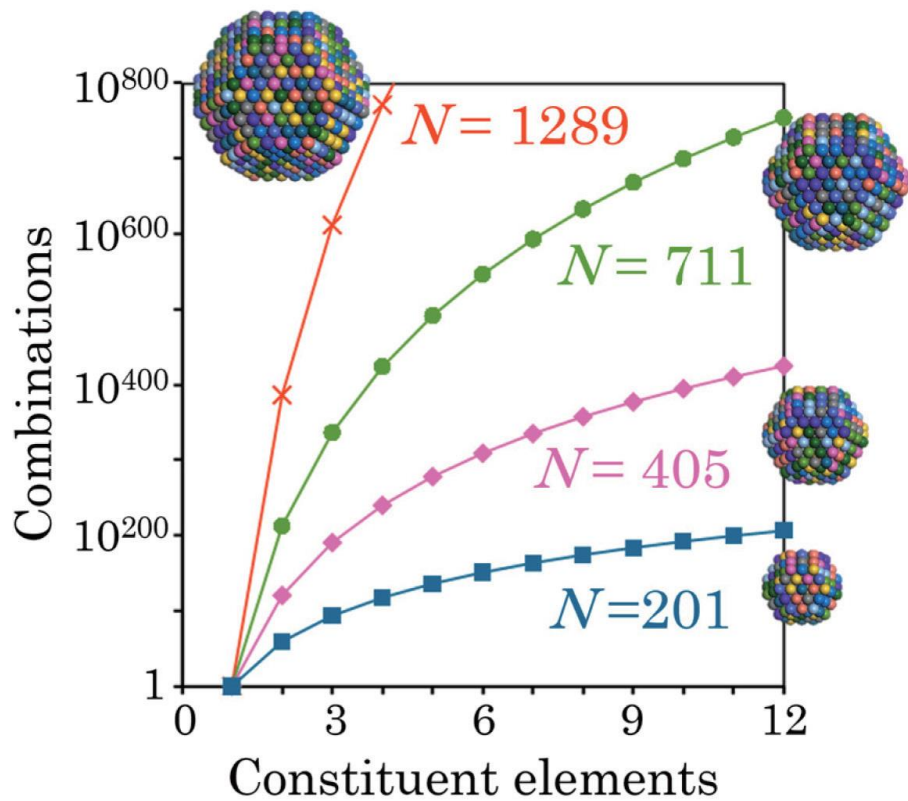
# AuPt alloy NPs: Role of Size and Composition

*Long heating at constant temperature of AuPt alloy NPs,  $T_{max} = 1100\text{ K}$*

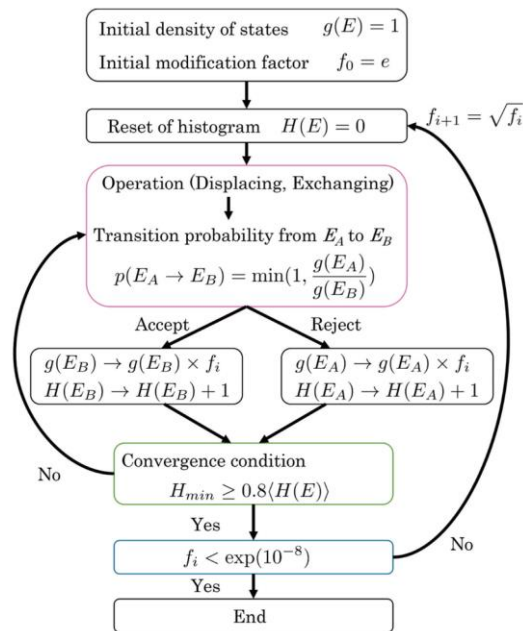
$R=12, f=0.5$	$R=25, f=0.2$	$R=25, f=0.5$	$R=25, f=0.8$
			
			
			

**AuPt alloy NPs upon long heating at 1100 K – partial segregation is observed depending on size, but also on composition  
(it is more probable at  $f=0.5$  for all the sizes)**

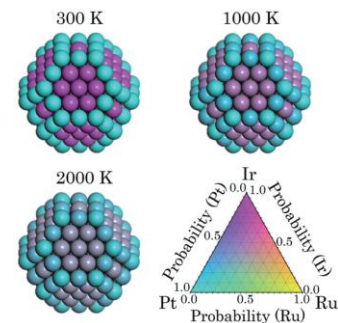
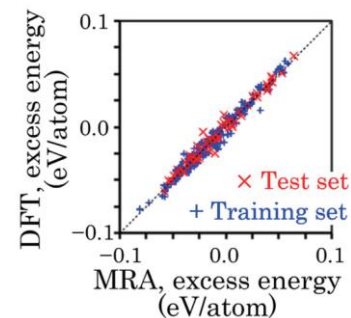
# Wang-Landau Monte Carlo for Probing Thermodynamic Stable Configurations vs DFT based Machine Learning



Number of configurations of alloy NP models consisting of 201, 405, 711, and 1289 atoms

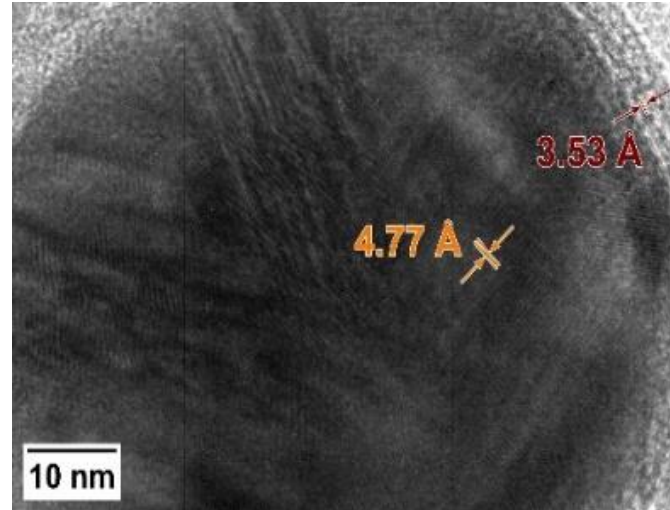
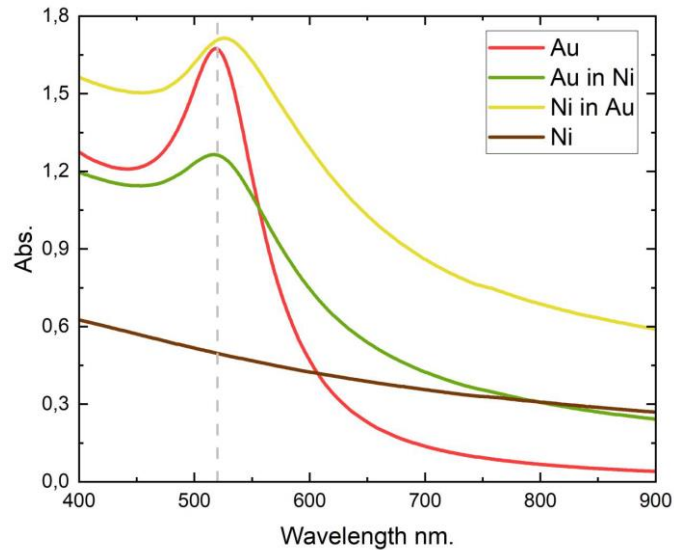


## Machine Learning



Y. Nanba *Journal of Computer Chemistry*, Vol. 9, 2022-0013 (2023)

# The Role of Chemistry in the Experiments with Ultra-Short Laser Pulses (Au-Ni NPs in Acetone)



**Carbon was found on the surface of Ni NP**

**Ni NP oxidation was found**

*Plasmonic properties of Au-Ni nanoparticles, LP3, Marseille*

*T. Itina et al, Lase 2025, SPIE*

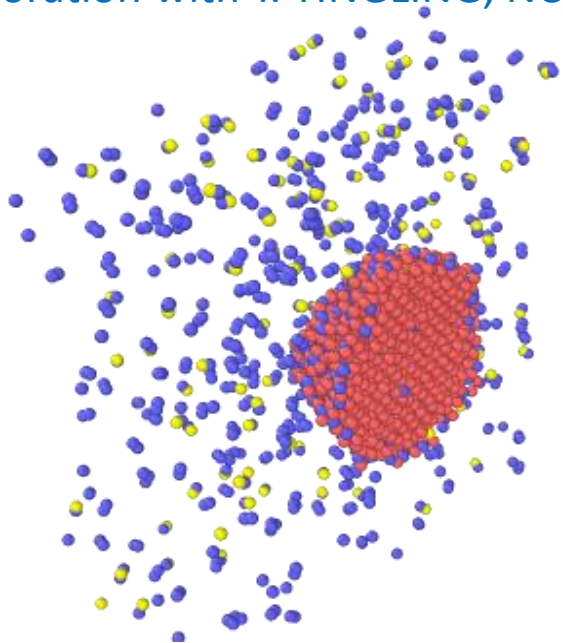
Ni and Au NPs were produced via femtosecond laser ablation in acetone (150  $\mu$ J, 490 fs, 10 kHz repetition rate).

HR-TEM images of Ni NPs and size distribution of Ni-Au NPs after 3 hours of co-fragmentation

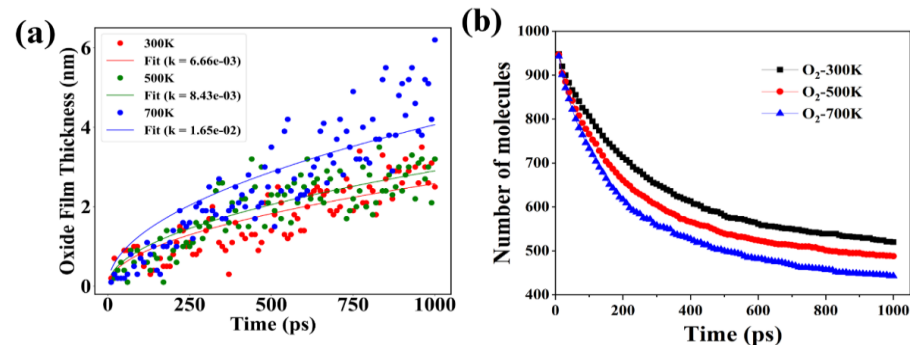
# ReaxFF MD : Ni NP in O<sub>2</sub> and C

Ni nanoparticle in a mixture of oxygen (blue) and carbon (yellow) at the beginning of the simulation (a) and upon heating to 1800 K during 12.5 ps (b). One can clearly see chemical reactions in the system and particularly at the surface.

ReaxFF model for Ni NP reactions  
with oxygen and carbon,  
(collaboration with Y. YINGLING, NC, USA)



Ti in O<sub>2</sub> after fs laser treatment



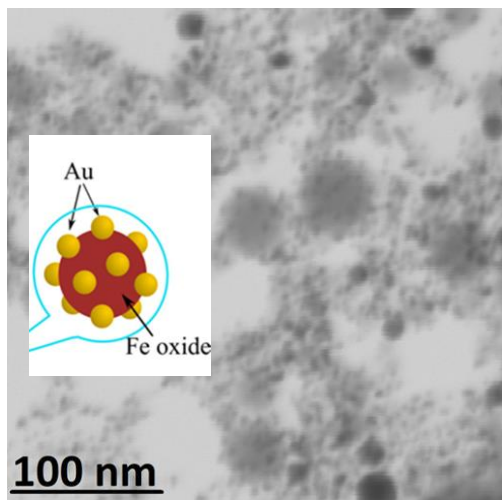
*I.S. Omeje et al. 2025, Surfaces and interfaces*

*For more details concerning  
oxidation of Ni NP see:  
poster by A. TOULIL et al EMRS-2025*

**Typical film thickness formed on metal surface inversely correlates to the change in the number of molecules at different maximum temperatures.**

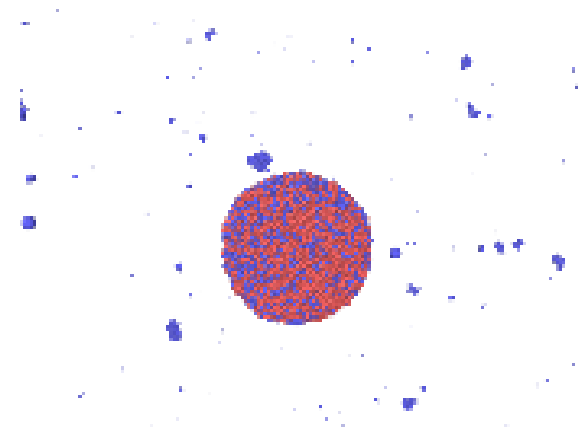
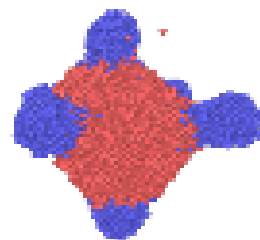
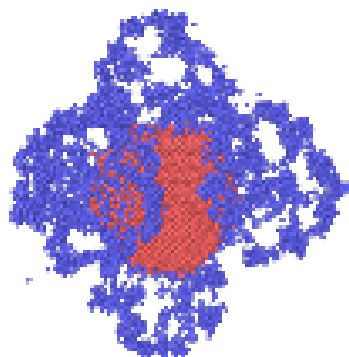


# Complex Nano-Objects Formation by Laser Co-Ablation

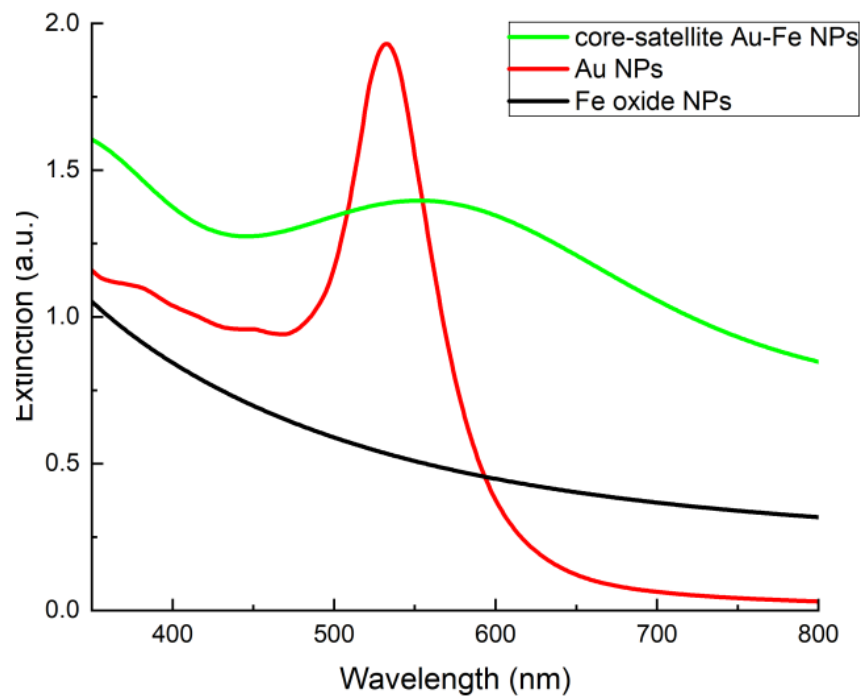


STEM image of nanostructures

obtained by mixing of negatively charged laser-ablated Au NPs and positively charged laser-ablated Fe oxide NPs. Right: Calculated extinction spectra of bare Au NPs (red line), Fe oxide NPs (black line) and core-satellite Au-Fe NPs (green line).

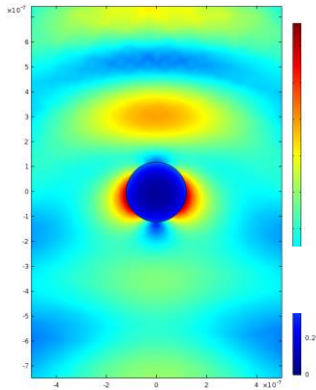


Raspberry-like, core-shells or alloys



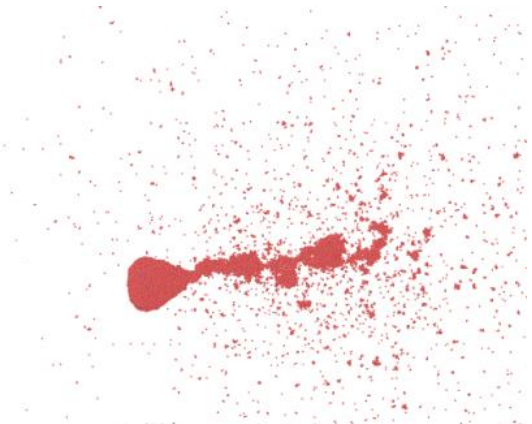
# Symmetry Breaking

Au NP in water



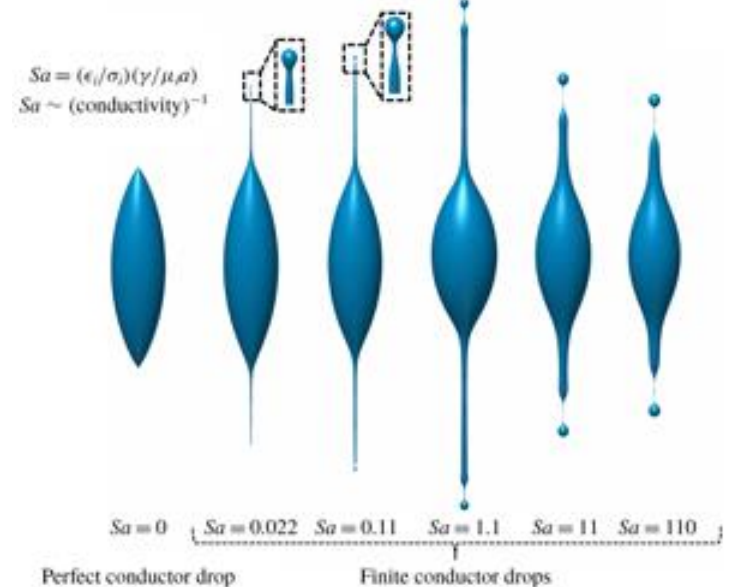
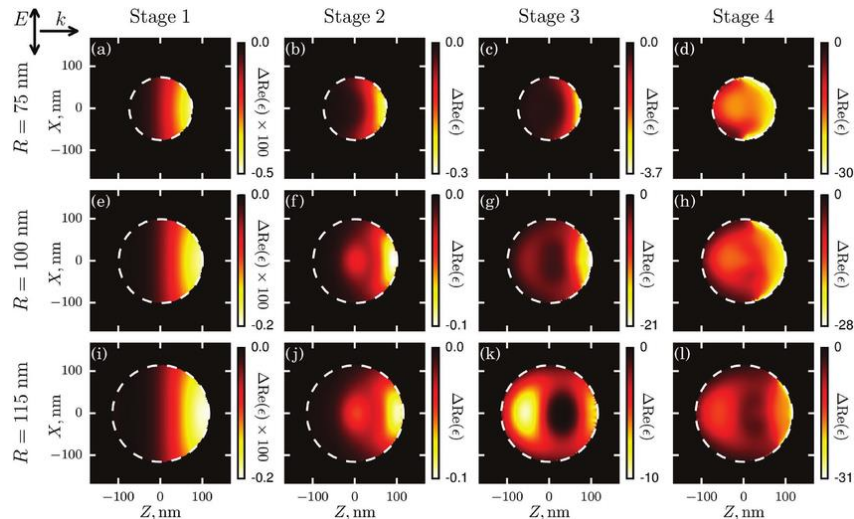
*Itina T.E, Nanoscale Adv 2024, 6, 5451*

Fluid instabilities



*Bhuyan, M. K., Soleilhac, A., Somayaji, M., Itina, T. E., Antoine, R., & Stoian, R. (2018). Scientific Reports, 8(1), 9665.*

Si NP



Ion Jets and Rayleigh break-up

*Journal of Fluid Mechanics, Volume 884, 10 February 2020, A31*

*Rudenko, A., Ladutenko, K., Makarov, S., & Itina, T. E. (2018). Nanoparticle. Advanced Optical Materials, 6(7), 1701153.*

# SUMMARY

**The results highlight the diverse strongly non-equilibrium phenomena induced by ultrashort pulses, from material ablation to modifications of nanoparticles.**

- Nanoparticles can be directly ejected from targets by laser pulses
- Nanoparticles can be either sintered or fragmented
- Laser pulses do induce nanoparticle vibrations prior to fragmentation
- Change in Gibbs energy is important (size, concentration, T, fraction of elements)
- In liquids, bubbles may affect nanoparticles and vice versa
- Better understanding and control over chemical reactions can be achieved by using ReaxFF MD and DFT.

**These findings pave the way for the development of multifunctional nanoparticles with potential applications in catalysis, magneto-optical devices, and biomedicine.**

## ACKNOWLEDGEMENTS

We acknowledge the financial support of Université Jean Monnet and CNRS, as well as CINES of France for the computational resources needed for large-scale simulations.

**Thank you very much  
for your attention!**

[tatiana.itina@univ-st-etienne.fr](mailto:tatiana.itina@univ-st-etienne.fr)