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Simulation of molecular formation dynamics in laser-induced plasmas with ReaxFF

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SCAI-RAC-Workshop

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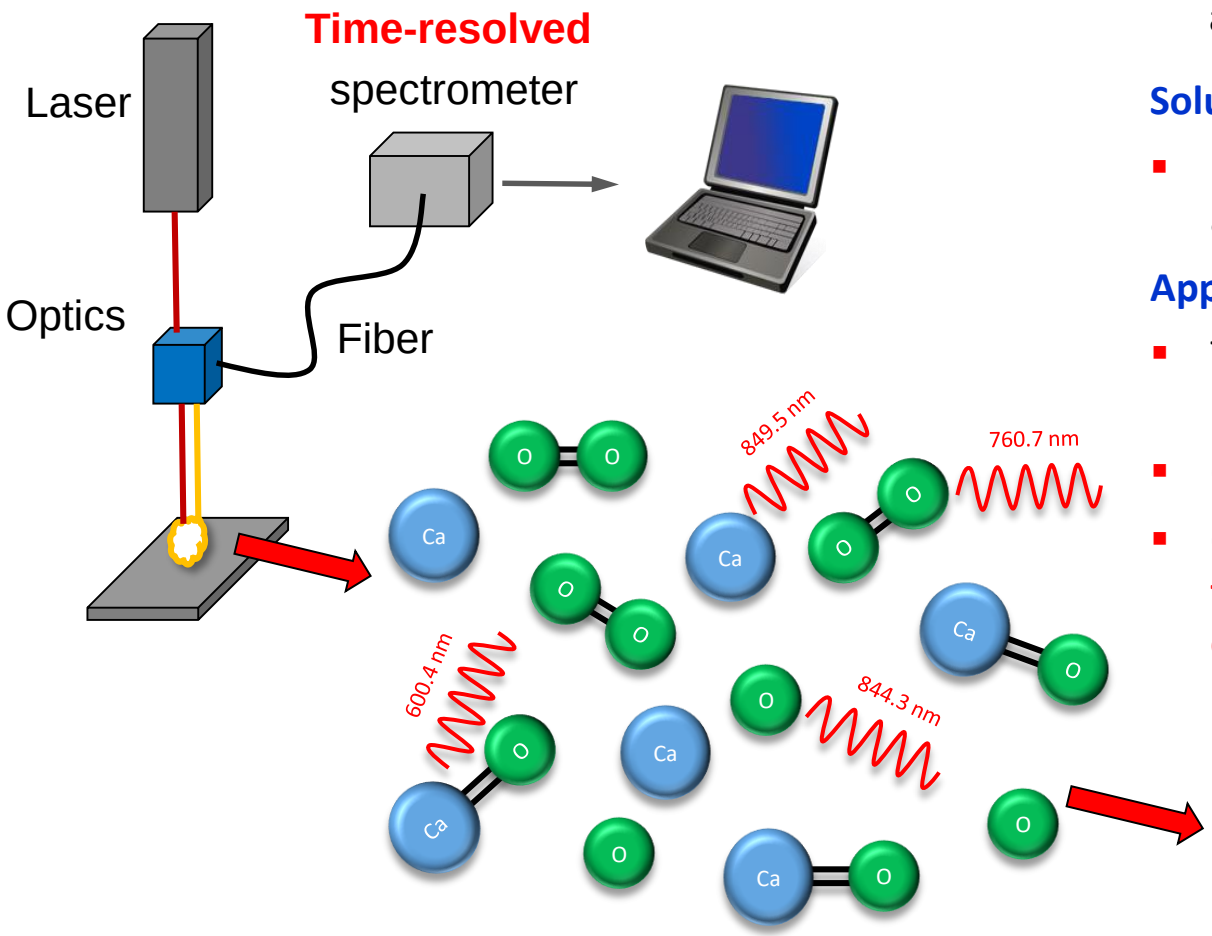
Background LIBS

LIBS: Laser Induced Breakdown Spectroscopy



Problem

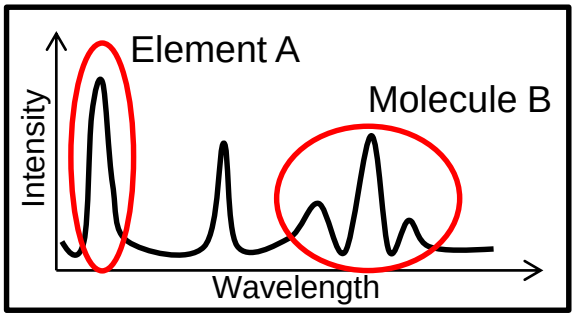
- Weak emission intensities of some atoms & ions for quantification

Solution for specific molecules

- Molecular band emission >> atomic & ionic line intensities

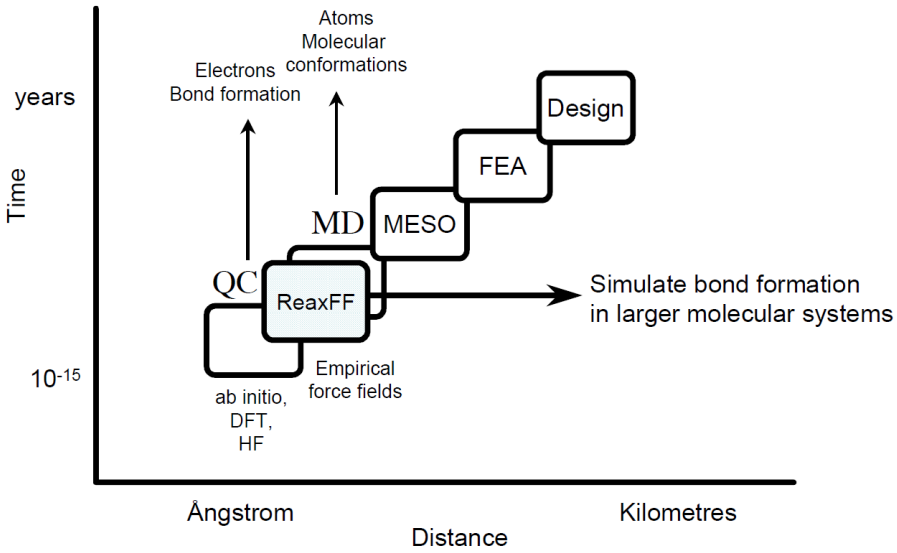
Approach

- Temperature determination of laser-induced plasma
- Optimizing experimental parameters
- Correlation of **simulated species formation** & **experimental species emission**



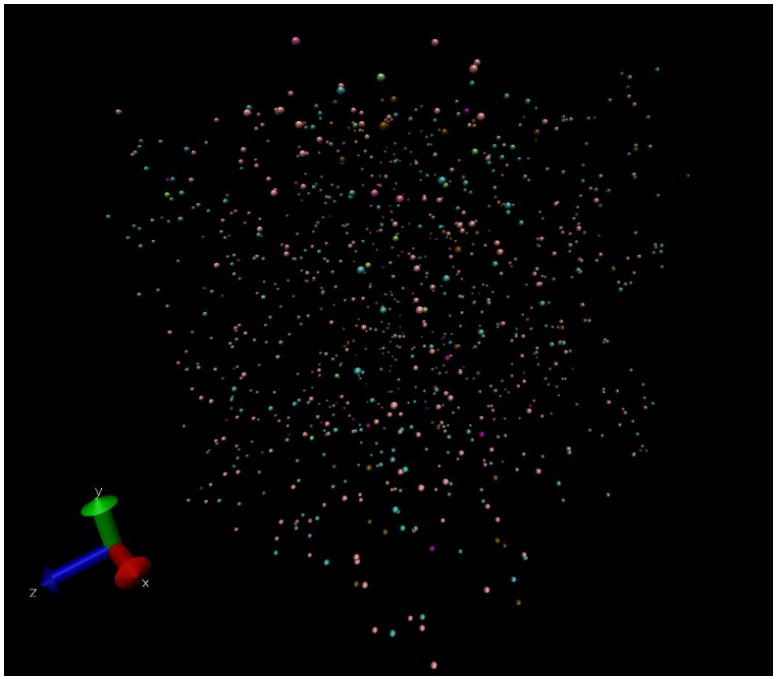
"Spectral fingerprint"

Reactive ForceField (ReaxFF)



Adri van Duin: ReaxFF User Manual (2002)

Typical starting system containing Ca and O (10,000K)



- Method for the simulation of molecular dynamics on atomistic scales
- Formation and destruction of chemical bonds
- Accordance with QM and Law of Mass Action (LMA)
- Radiation losses compensated by thermostats

Simulation inputs

- ForceField
- Starting system (6000 atoms)
- $v_{Ca} \approx 2500$ m/s

ReaxFF: Temperature ramp simulations

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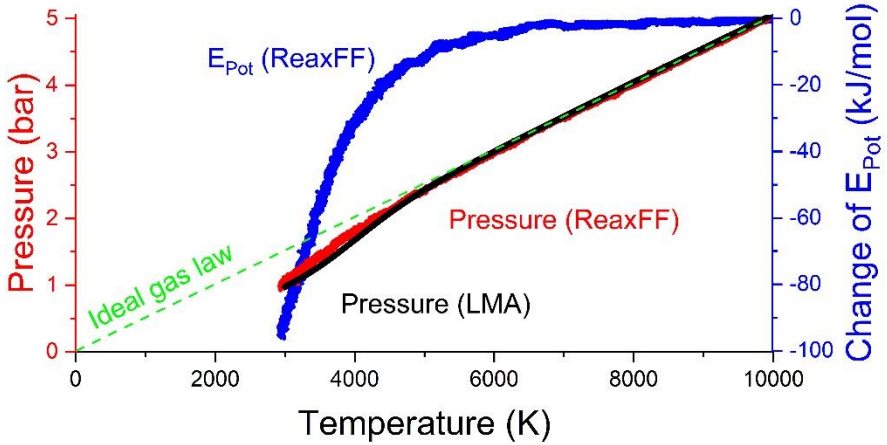
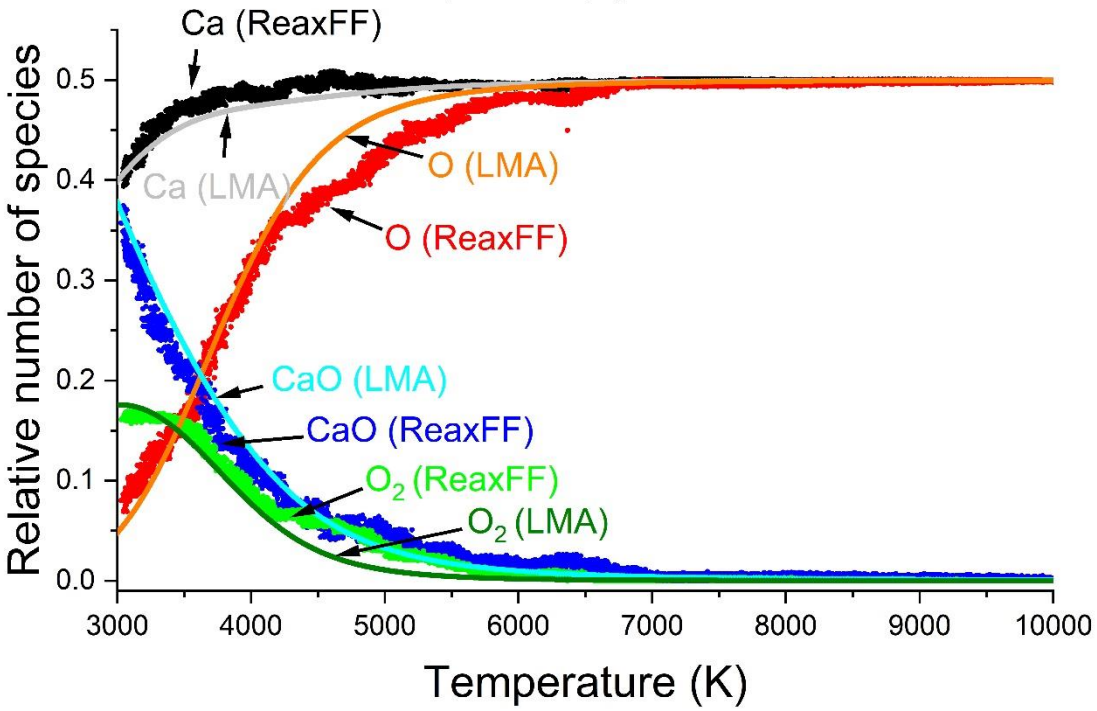
Profile of thermodynamic parameters

- T, E_{pot}, E_{kin}, p, F, v, xyz…
  (10^8 time steps)



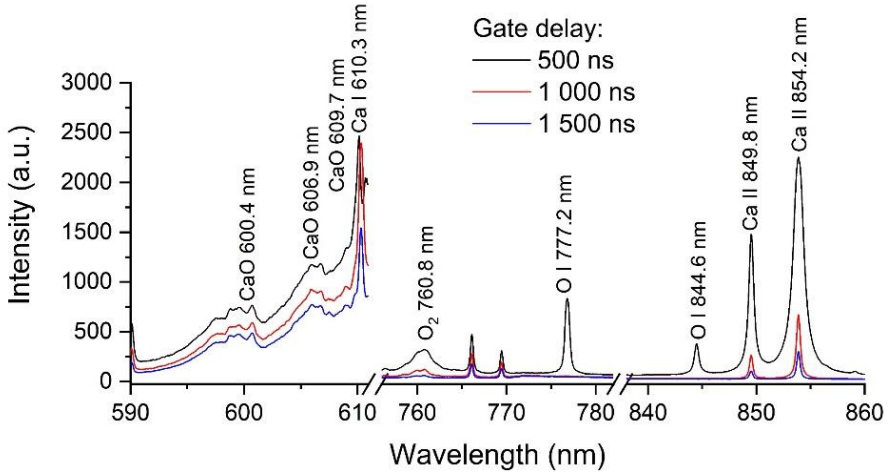
Profile of molecular formation

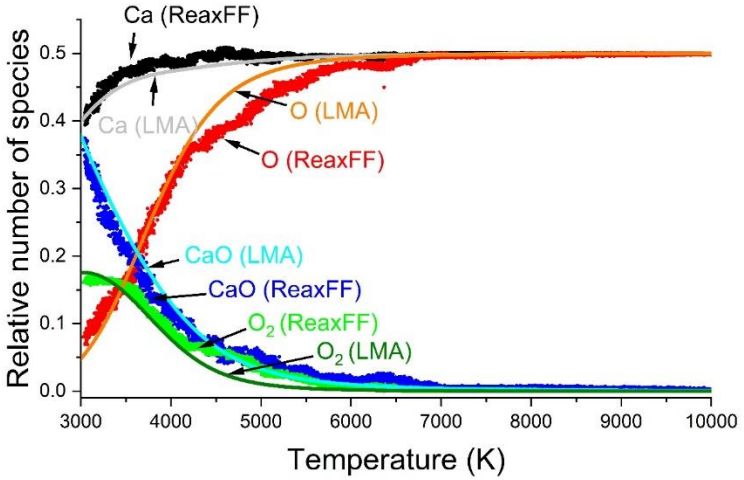
- Reaction rates
  - Lack of reactants & reactions
  - Maximum of formation
  - Particle tracking



T. Dietz, P. Kohns, G. Ankerhold, Diagnostics and simulations of molecular formation in laser-induced plasmas, Spectrochimica Acta Part B **148** (2018) 51-59

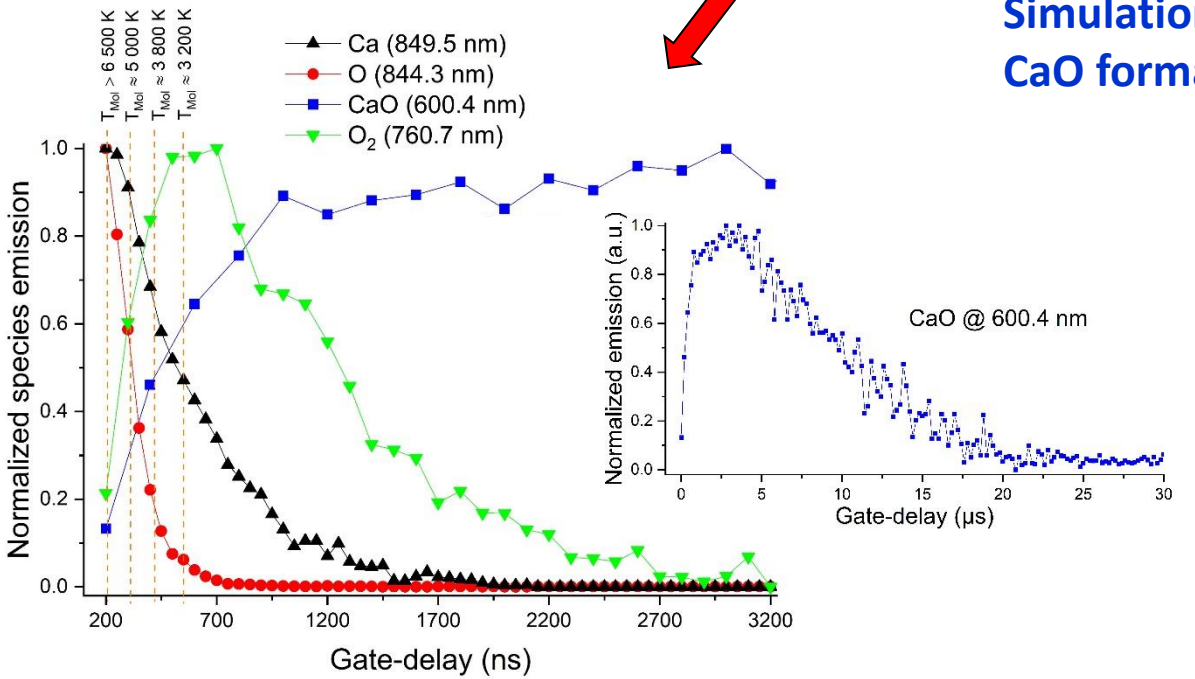
LIBS measurements





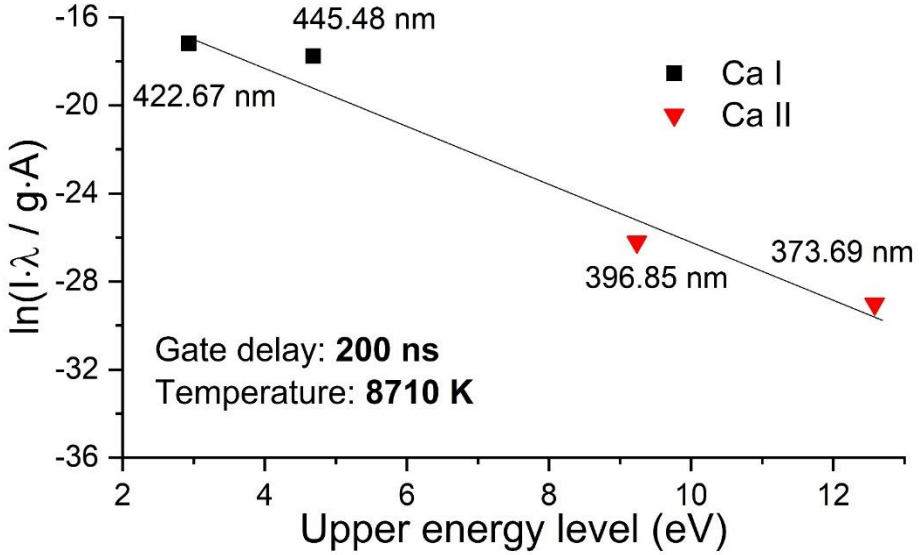
Time resolved spectra of CaO

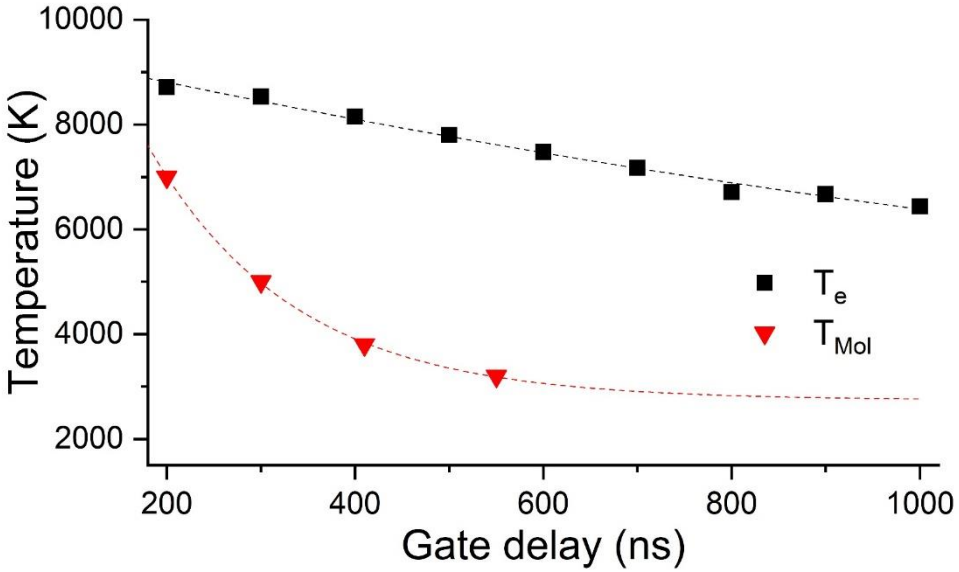
Simulation of CaO formation



Temperature determination

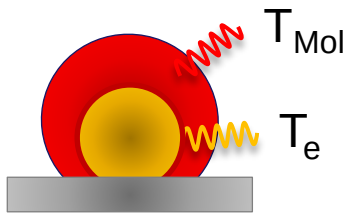
Plasma temperatures





Electron temperature by Saha-Boltzmann method

- Assumption: Local thermodynamic equilibrium required



$T_{Core} > T_{Periphery}$

Molecular temperature estimation of LIBS plasma using ReaxFF simulations & species emission

Summary

- ReaxFF can give a better understanding of **molecular formation** in LIBS plasmas
- Determination of local electron & molecular **plasma temperatures**
- **Designing** & **optimizing** LIBS experiments for material analysis

Funded by

Federal Ministry for Economic Affairs and Energy

T. Dietz, J. Klose, P. Kohns, G. Ankerhold, Quantitative determination of chlorides by molecular LIBS, Spectrochimica Acta Part B (under review)