EUCALL Workshop on Theory and Simulations of Photon-Matter Interaction

ELI-ALPS, Szeged, Hungary
July 7, 2018

# Incomplete Workshop Summary

European XFEL

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 654220

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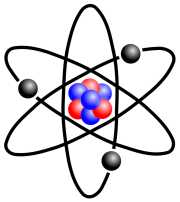
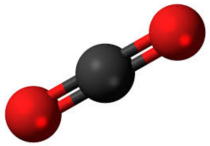
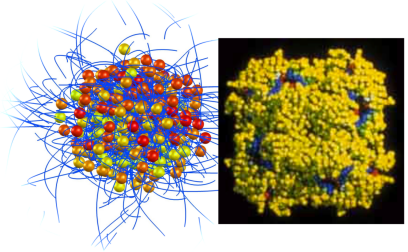
# Finite systems in intense fields



- Correlations (beyond HF-S)
- Numerical treatment of complex ionization dynamics
- Inclusion of more transitions (e.g. electron impact on exotic ions)
- Nonlinearities, interference between transitions of similar cross-sections?
- Model potentials (e.g. for HHG generation)



- Charge transfer and ionization dynamics in HFS (well defined but numerically expensive)
- DFT simulations of luminescence in perovskites



- (TD)SE not practicable
- (TD)DFT
- PIC for finite systems
  - atomic physics?
  - collisions, correlations
  - Quantum dynamics (so far only very simple cases)

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# Extended systems, in particular WDM (Γ~1, T/TF ~1)

- Non-perturbative, time-dependent treatment necessary including quantum effects and correlations
- DFT:
  - Temperature dependent XC functionals (WDM), currently only LDA
  - Excited states?
  - e-e correlations?
- Beyond (TD)DFT methods (NEGF) → how to approximate self-energy, not always well defined, transferrability of self-energy hard to achieve
- Effective Hamiltonians
  - Tight binding, Hubbard model → limited transferrability, parametrizations must come from ab-initio
- Direct models
  - BMA, BMA+LFC, need benchmarking against ab-initio
- Bandstructure “remainders” in WDM creation
- Ab-initio treatment of solids interacting with focussed lasers (no PBC applicable)

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# Advanced techniques

- Bridge/interpolate condensed matter to hot dense matter (via WDM)
- Time dependent description of ultrafast phenomena including quantum effects **and** correlations
- → Nonequilibrium Green Functions and diagram technique (self-energy, vertex term, self-consistent schemes → GW (and beyond)). Controllable?
- Similar techniques in QED (perturbative, non-perturbative)
  - E.g. radiation reaction problem ↔ how to pick the right terms in Σ in MBPT
  - QED processes in PIC → in-medium QED
- Conjecture: correlations weaken at high intensity → where exactly are the limits, counterexamples exist, e.g. inverse bremsstrahlung
- **Strong need for method development.**

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# Challenges in the light of current experimental research and future developments

- Attosecond science, HHG
  - Separation of harmonics → polarization control + quasi-phasematching
  - Predictive simulations difficult
- PIC codes:
  - Atomic physics
  - Collisions, improved collision frequencies → straightforward, but implementation into complex PIC codes involved
  - finite systems
  - noneq. QED radiative cross sections
- Diagnostics of HED imaging experiments
  - advanced reconstruction techniques needed,

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# Future developments at light sources and challenges for theory

- XUV/X-FELS
  - Polarization control
  - MHz rep rate and beyond → CW mode
  - What intensities & wavelengths ultimately achievable?
  - Proposals for new FEL schemes and beamlines are developed **now,** fundamental science should drive these
- OLs
  - Approaching the Schwinger limit
  - QED cascades → direct impact on safety considerations
  - Implementation of QED in PIC → treat plasma effects on same footing

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# Please

- Send us your presentations → workshop website
- Fill our survey, give feedback
- Keep in touch
- Suggest follow up events, spread the word
- Have a safe trip home!

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# Thanks go to ...

- All speakers for excellent contributions
- ELI-ALPS for the hospitality
- ELI-DC for the local organization
- Graham
- EUCALL for financial support

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# ... and YOU

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