Theoretical Modeling of Ultrafast Phase Transitions from the Femtosecond to the Picosecond Scale

S. Mocatti, A. Corradini, G. Volpato, X. Zhu, G. Marini, P. Cudazzo and M. Calandra

MATERIALS THEORY

erc European Research Council

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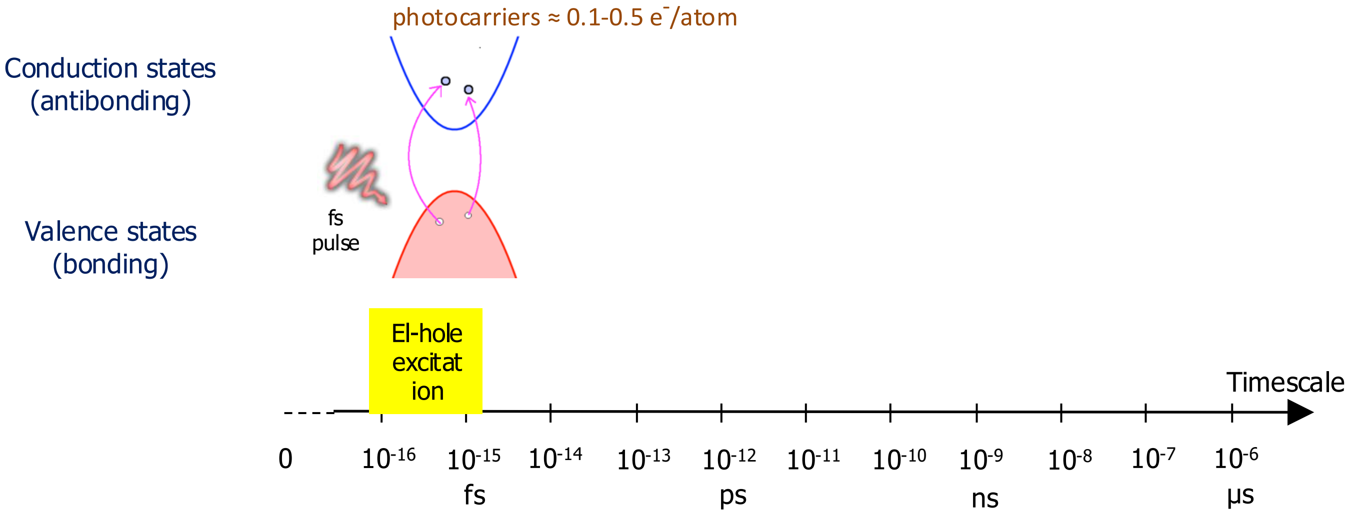
Ultrafast phase transitions in extended systems



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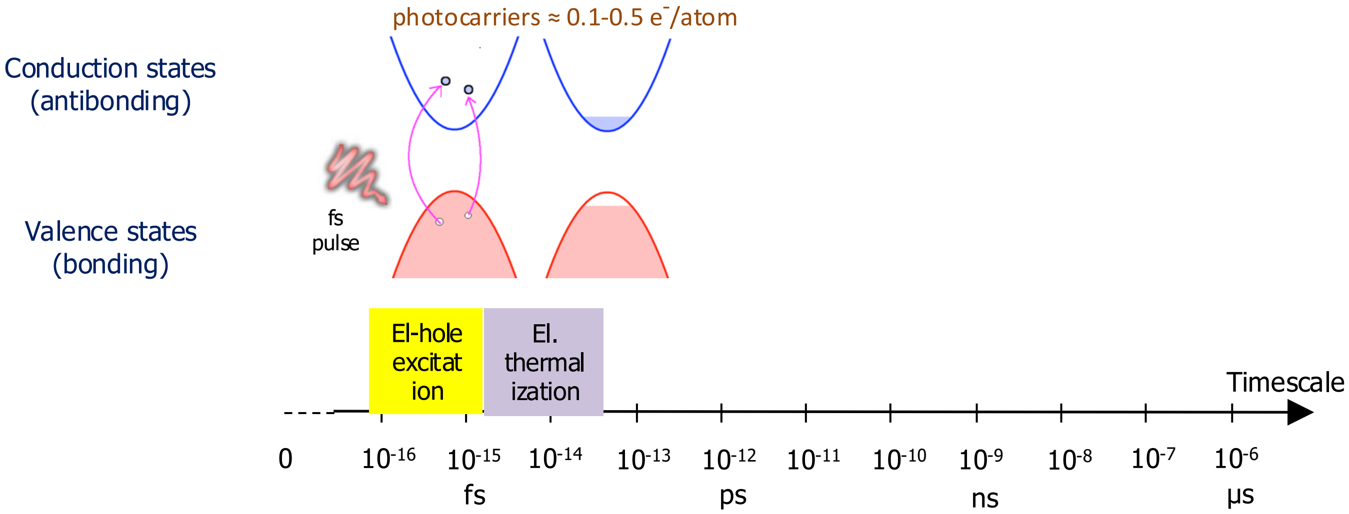

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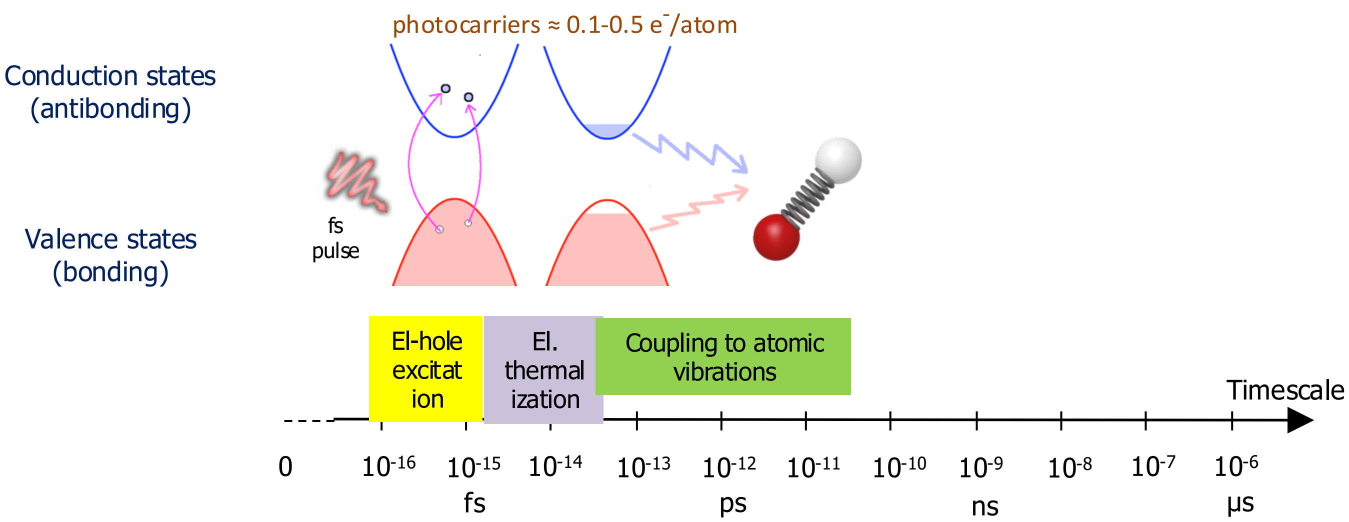

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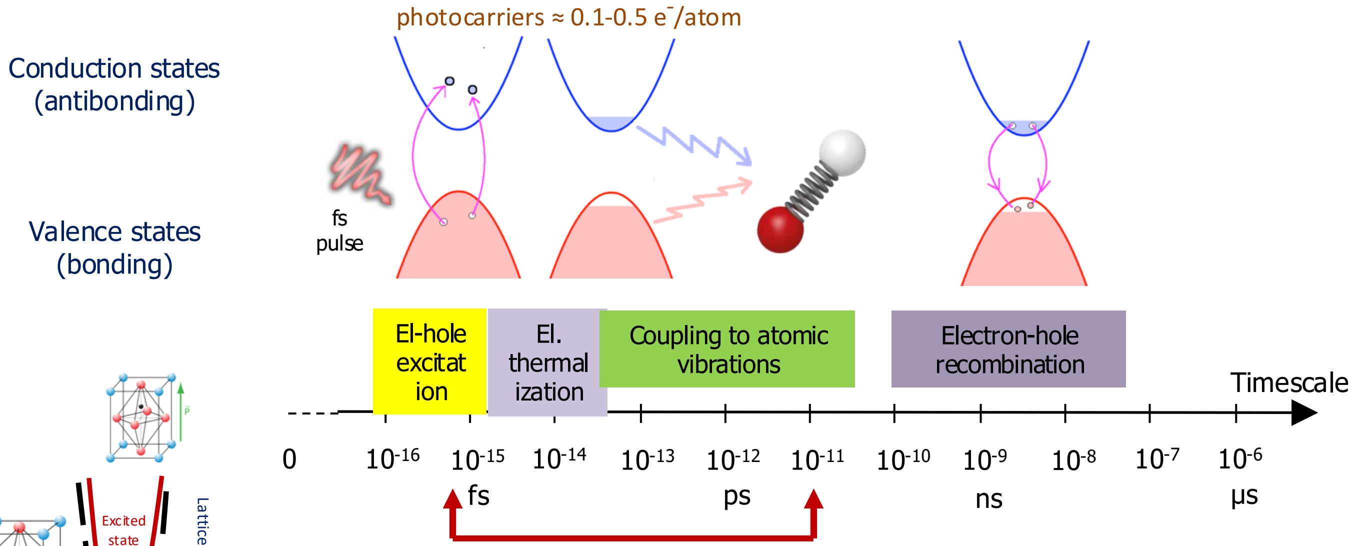
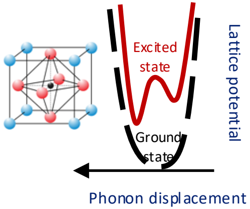




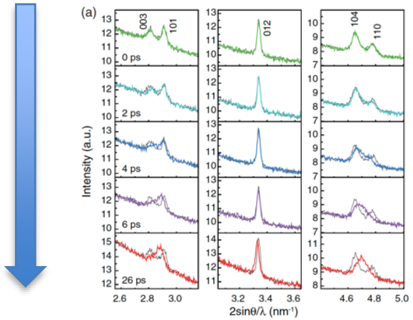
The large occupation of antibonding states triggers phase transitions.

We are interested in the photocarriers thermalization and in the phase transitions occurring after electron thermalization.

How do we prove the occurrence of a phase transition ?

- Ultrafast diffraction via X-ray free electron laser

time



GeTe

E. Matsubara *et al.* PRL **117**, 135501 (2016)

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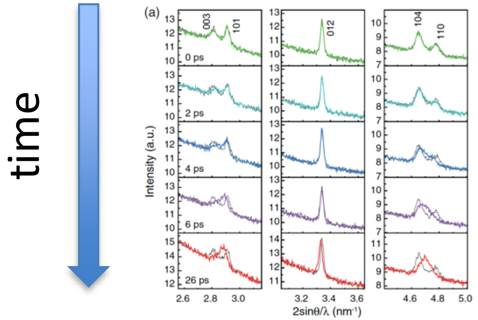
GeTe



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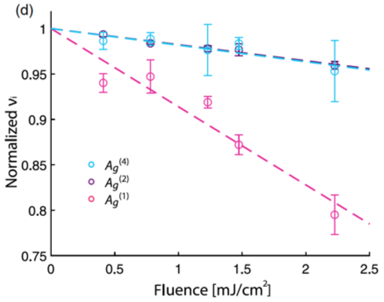
- Raman active modes displacive excitation of coherent Phonons (reflectivity oscillations)

SnSe



Huang *et al.* PRX **12**, 011029 (2022)

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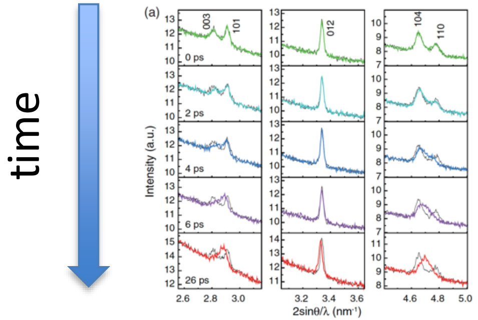

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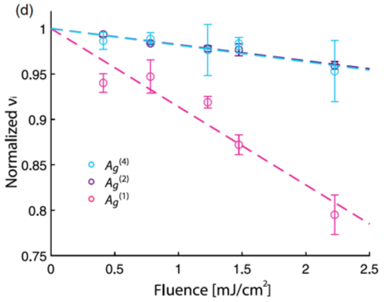
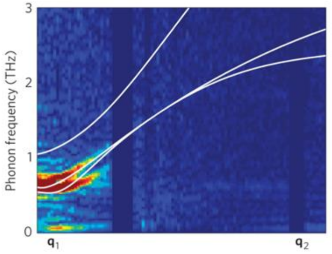


SnSe

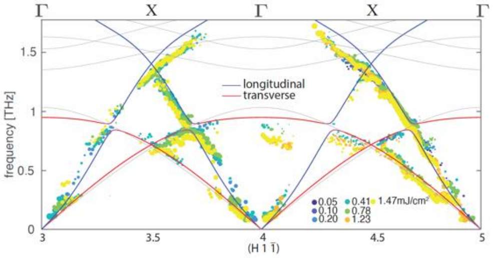
Huang *et al.* PRX **12**, 011029 (2022)

- Phonon dispersion via fs thermal diffuse scattering

Bulk Ge



M. Trigo *et al.* Nat. Phys 9, 790 (2013)



SnSe

Huang *et al.* arXiv:2301.08955v1

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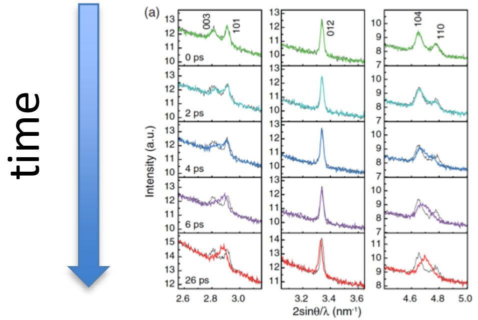

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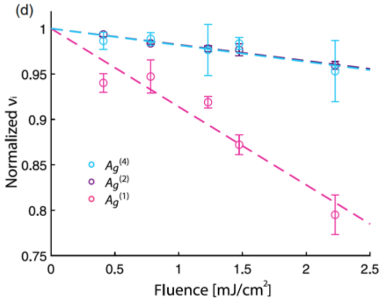

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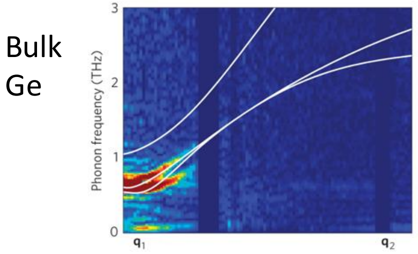

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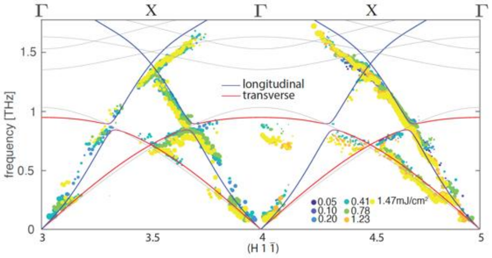
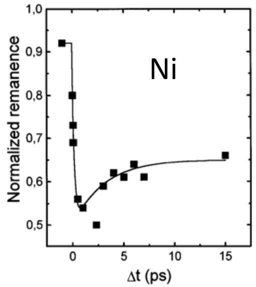


Huang *et al.* arXiv:2301.08955v1

- Magnetism via ultrafast MOKE



E. Beaurepaire *et al.* PRL **76**, 4250 (1996)

What are the tipical fluences and the number of photoexcited carriers ?

- Single-shot damage threashold depends on the materials and, even more, on the experimental setting.

SYSTEM	Fluence used (mJ/cm^2)	Photocarriers/cell	Damage threashold (mJ/cm^2)
VO_2 [1,2]	25	0.31	65
GeTe [3,4]	7-20	0.1-0.36	35-50 (amorphysation)
SnSe [4,5]	2.2 (in vacuum)	0.3	>3 (caveat: T=300, inefficient heat diss.)
SnSe [6]	13.2 (on top of diamond)	1.8	

Sample damage is mainly related to difficulties in heat dissipation.
Different set up show very different damage threashold (see later)

[1] A. Cavalleri *et al.* PRL 87, 237401 (2001).
[2] S. Wall *et al.* Science 362, 572 (2018)
[3] J. Hu *et al.* ACS Nano 9, 6728 (2015)
[4] E. Matsubara *et al.* PRL **117**, 135501 (2016)
[5] Huang et al. PRX 12, 011029 (2022)
[6] B. J. Dringoli *et al.* arXiv:2212.12498

How to simulate the laser pumping + the photocarriers dynamics (short times).

$$\hat{H}(t) = \hat{H}_{\rm el}^{\rm sp} + \hat{H}_{\rm el-el} + \hat{H}_{\rm harm} + \hat{H}_{\rm el-ph} + \hat{H}_{\rm ph-ph} + \hat{H}_{\rm laser}(t)$$

Single particle electrons

Harmonic phonons

Electric field

$$\hat{H}_{\rm laser}(t) = \sqrt{2}\sum_{\mathbf{k}n,m} \mathbf{E}(t)\mathcal{D}_{n,m}(\mathbf{k})\,\hat{\mathbf{c}}^{\dagger}_{\mathbf{kn}}\hat{\mathbf{c}}_{\mathbf{km}}$$

Dipole matrix element

How to simulate the laser pumping + the photocarriers dynamics (short times).

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The non-equilibrium average of an operator reads

$\langle \hat{\mathcal{O}} \rangle_t = \mathrm{Tr}[\hat{\rho}(t)\hat{\mathcal{O}}]$ where $\hat{\rho}(t)$ is the finite T manybody density matrix

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Stefanucci *et al.*, PRX 13, 031026 (2026)
S. Mocatti *et al.* npj comp. Materials (2026)
10.1038/s41524-026-02104-y

The operators we are interested in are

$f_{\mathbf{k}n}(t) = \langle \hat{c}^\dagger_{\mathbf{k}n} \hat{c}_{\mathbf{k}n} \rangle_t$ Electronic occupation

$n_{\mathbf{q}\nu}(t) = \langle \hat{a}^\dagger_{\mathbf{q}\nu} \hat{a}_{\mathbf{q}\nu} \rangle_t$

Phonon occupation

$p_{\mathbf{k}nm}(t) = \langle \hat{c}^\dagger_{\mathbf{k}m} \hat{c}_{\mathbf{k}n} \rangle_t \quad \text{for} \quad n \neq m.$

interband polarization

+ coherent phonons, exciton melting..

How to simulate the laser pumping + the photocarriers dynamics (short times).

Semiconducting Bloch Equations

$$\Omega_{\mathbf{k}nm}(t) = \sqrt{2}\mathbf{E}(t) \cdot \langle \psi_{\mathbf{k}n} | \hat{\mathbf{r}} | \psi_{\mathbf{k}m} \rangle$$

$$\frac{df_{\mathbf{k}n}(t)}{dt} = 2 \, \mathrm{Im} \left[\sum_{m \neq n} \Omega_{\mathbf{k}nm}(t) \, p_{\mathbf{k}mn}(t) \right] + \mathcal{I}^{ee}_{\mathbf{k}n}(t) + \mathcal{I}^{ep}_{\mathbf{k}n}(t)$$

$$\frac{dp_{\mathbf{k}nm}(t)}{dt} = -i \Big[[\varepsilon_{\mathbf{k}n}(t) - \varepsilon_{\mathbf{k}m}(t)] \, p_{\mathbf{k}nm}(t) + [f_{\mathbf{k}m}(t) - f_{\mathbf{k}n}(t)] \, \Omega_{\mathbf{k}nm}(t) \Big]$$
$$-i \Big[\sum_{m' \neq m} \Omega_{\mathbf{k}nm'}(t) p_{\mathbf{k}m'm}(t) - \sum_{n' \neq n} \Omega_{\mathbf{k}n'm}(t) p_{\mathbf{k}nn'}(t) \Big]$$
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$$\frac{dn_{\mathbf{q}\nu}(t)}{dt} = \mathcal{I}^{pe}_{\mathbf{q}\nu}(t) + \mathcal{I}^{pp}_{\mathbf{q}\nu}(t)$$

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Time dependent electronic structure (t dep. COHSEX+FM+ Coherent phonon)

$$\frac{dn_{\mathbf{q}\nu}(t)}{dt} = \mathcal{I}^{pe}_{\mathbf{q}\nu}(t) + \mathcal{I}^{pp}_{\mathbf{q}\nu}(t)$$

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Laser (pump)

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How to simulate the laser pumping + the photocarriers dynamics (short times).

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$$\frac{dn_{\mathbf{q}\nu}(t)}{dt} = \mathcal{I}^{pe}_{\mathbf{q}\nu}(t) + \mathcal{I}^{pp}_{\mathbf{q}\nu}(t)$$

Scattering integrals
(beyond RTA)

How to simulate the laser pumping + the photocarriers dynamics (short times).

Semiconducting Bloch Equations

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Damping

$$\frac{dn_{\mathbf{q}\nu}(t)}{dt} = \mathcal{I}^{pe}_{\mathbf{q}\nu}(t) + \mathcal{I}^{pp}_{\mathbf{q}\nu}(t)$$

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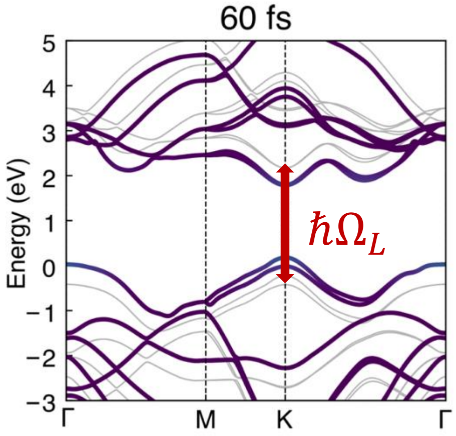
S Mocatti, G Marini, G Volpato, P Cudazzo, and M.C.
npj computational materials (2026), 10.1038/s41524-026-02104-y

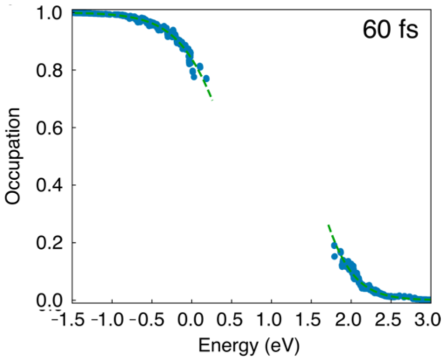
https://the-epiq-team.gitlab.io/epiq-site/

Ab-initio manybody real-time carrier dynamics

MoS_2 single layer

t=0
el. struct.





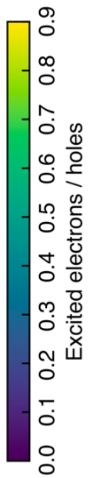
$$\mathbf{E}(t) = \mathbf{E}_0 \exp\left[-\frac{(t-t_0)^2}{2\Delta t^2}\right] \sin(\omega t)$$

$$\hbar\omega = 2.6\ \text{eV}$$

$$\Delta t = 5\ \text{fs}$$

$$t_0 = 15\,\text{fs}$$

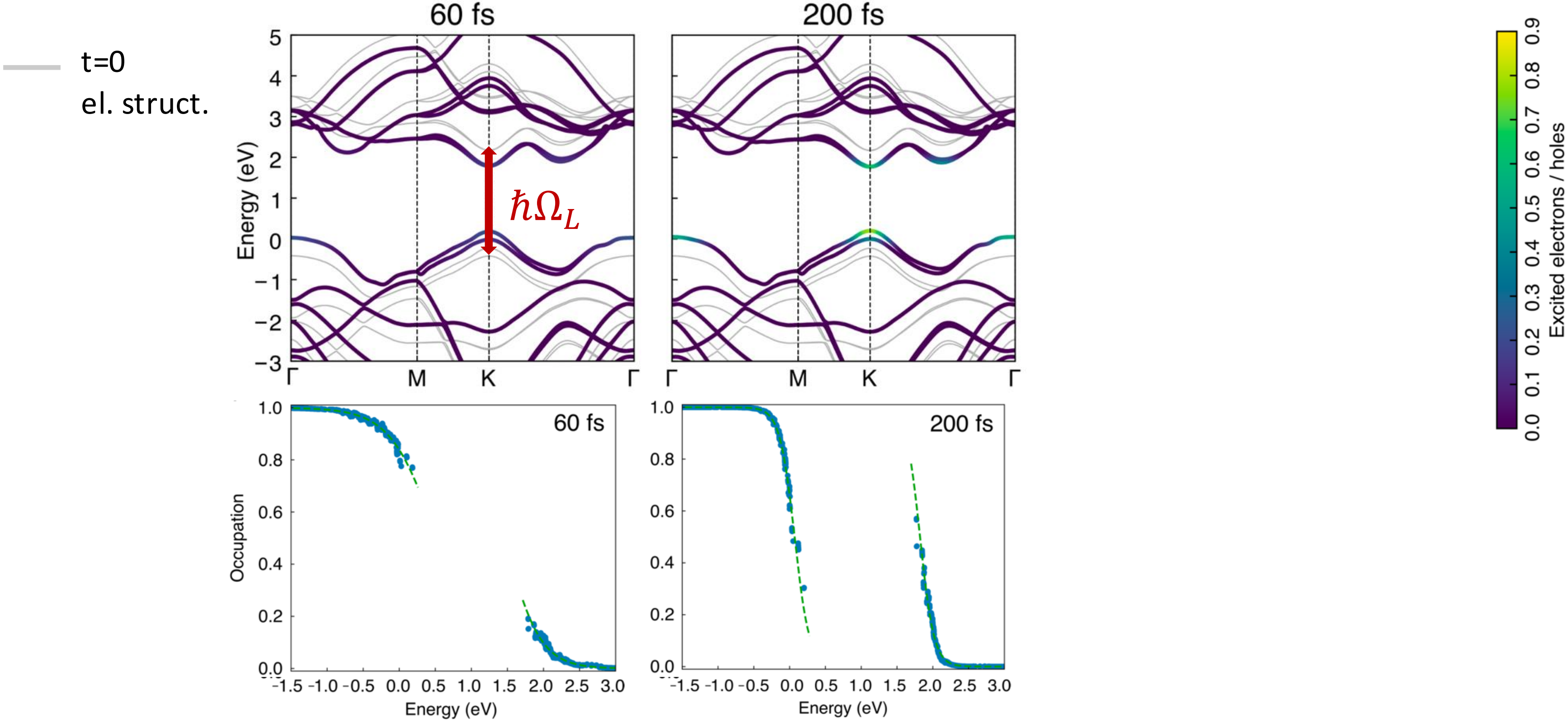
Polarized xy



At sufficient long times the photocarriers assume a two Fermi level distributions (electron-hole plasma)

Ab-initio manybody real-time carrier dynamics

MoS_2 single layer



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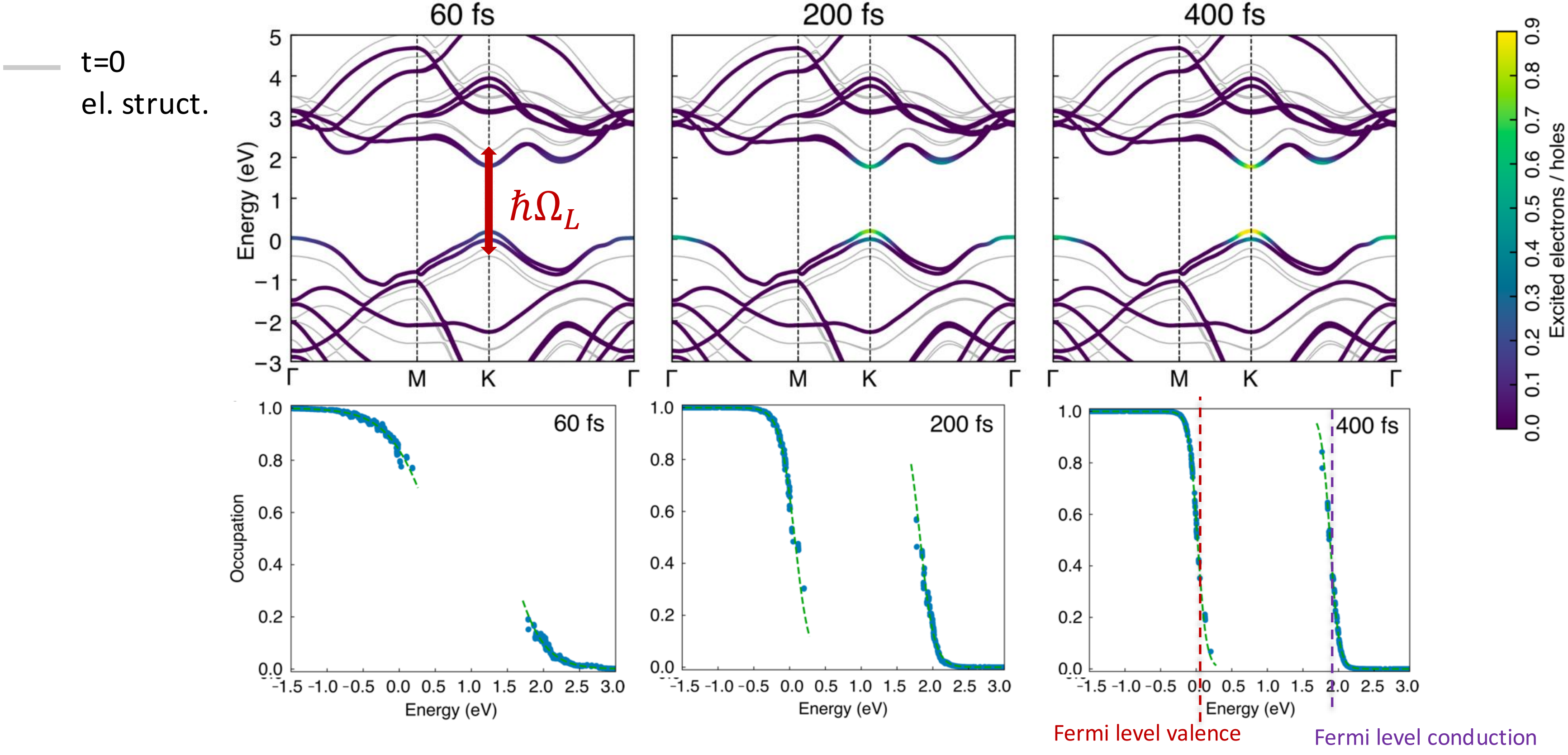

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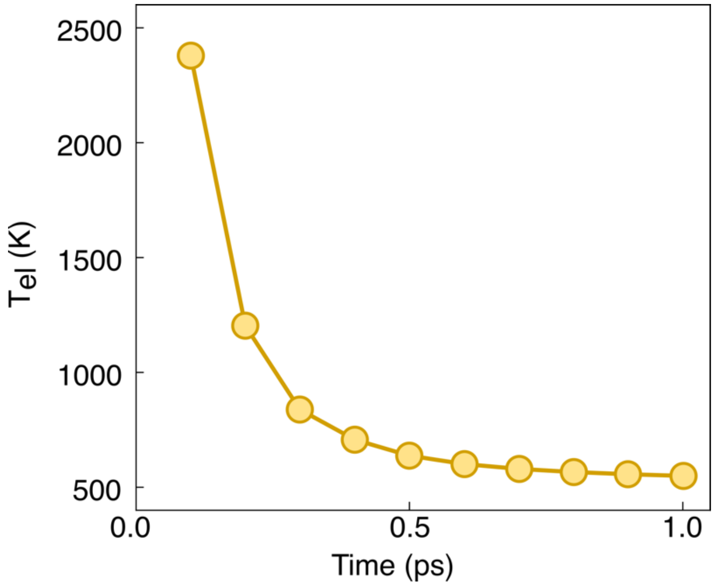
Evolution of electronic temperature

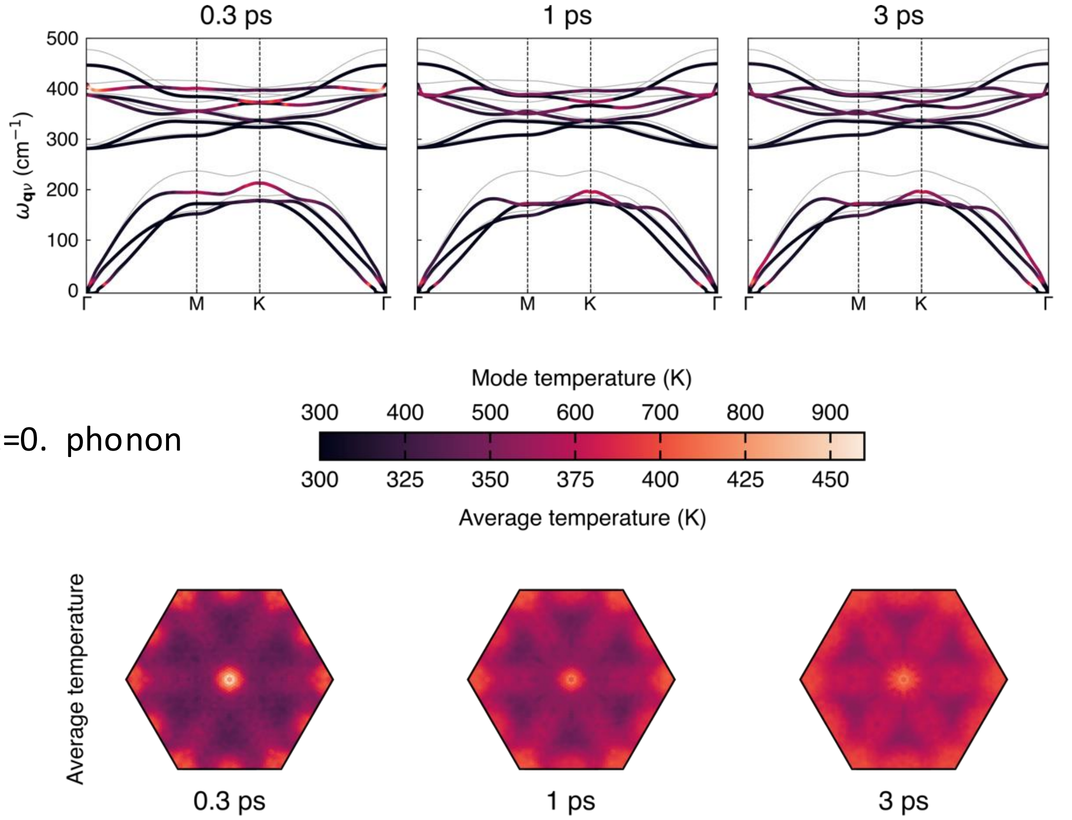
MoS_2 single layer



Heat transfer to the phonons

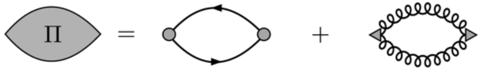
Phonon heating

MoS$_2$ single layer



t=0. phonon

t-dep of $\omega_{q\nu}$(t)

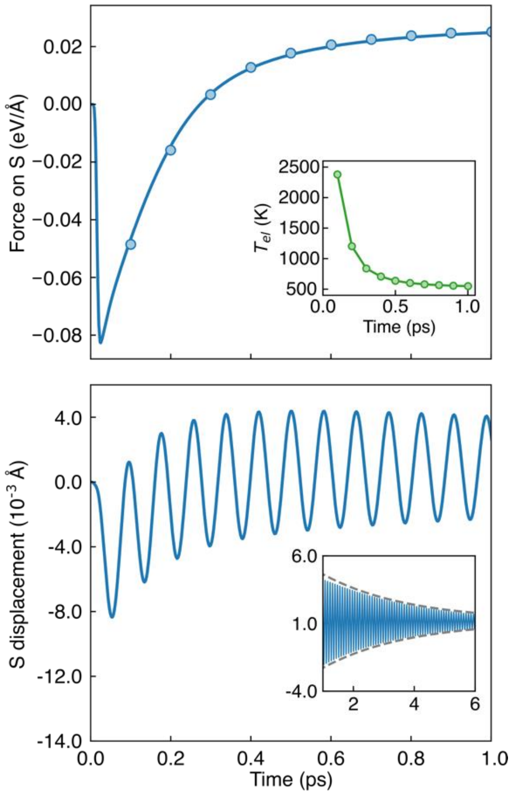


e-ph

Anharmonicity (third order)

Coherent phonons

MoS$_2$ single layer



A$_{1g}$ phonon mode

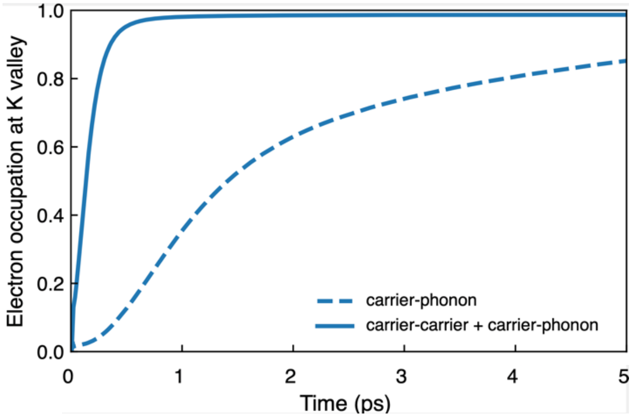
$$\frac{d^2 Q_\nu(t)}{dt^2} = -\omega_{\mathbf{0}\nu}^2 Q_\nu(t) - 2\Gamma_{\mathbf{0}\nu}\frac{dQ_\nu(t)}{dt} + F_\nu^{\mathrm{ep}}$$

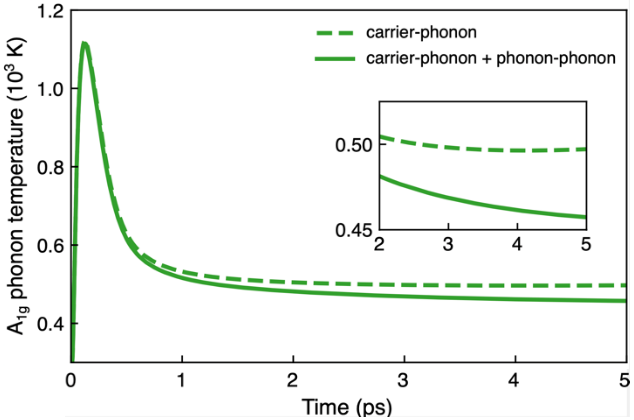
$$F_\nu^{ep}(t) = -\omega_{\mathbf{0}\nu}^0 \sqrt{\frac{2}{N}} \sum_{\mathbf{k},n} \Delta f_{\mathbf{k}n}(t) g_{nn}^\nu(\mathbf{k},\mathbf{0})$$

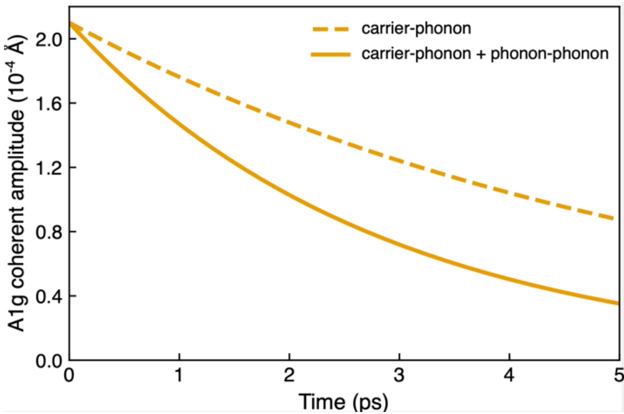
$$\Gamma_{\mathbf{0}\nu} = \Gamma_{\mathbf{0}\nu}^{\mathrm{ep}} + \Gamma_{\mathbf{0}\nu}^{\mathrm{ph-ph}}$$

Forces and damping from first principles

Crucial importance of treating all interactions on equal footing







Neglecting electron-electron: completely incorrect photocarriers relaxation times.

Electron-phonon scattering and phonon-phonon scatterings act a equal times.

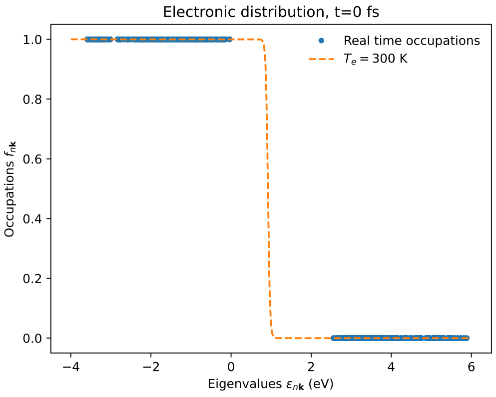
The coherent displacement of the A_{1g} mode is equally due to ph-ph and e-ph.

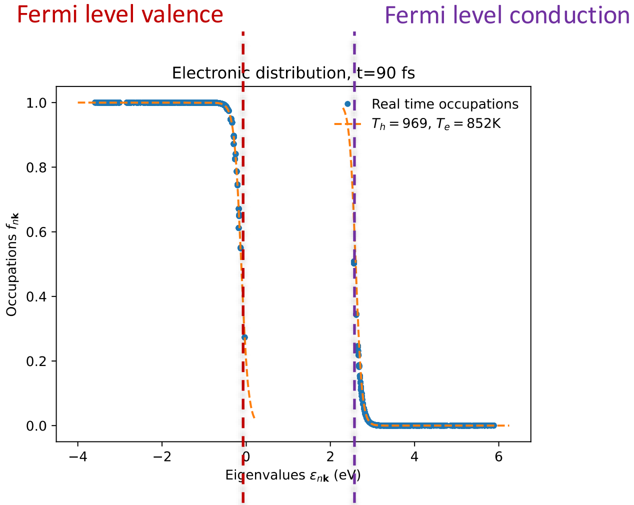



S Mocatti, G Marini, G Volpato, P Cudazzo, and M.C.
npj computational materials (2026), 10.1038/s41524-026-02104-y

Take home message from manybody calculations

- The electron-electron interaction is extremely efficient in thermalizing photocarriers.
- After few tens of fs the system is well described by a quasi equilibrium electron-hole plasma



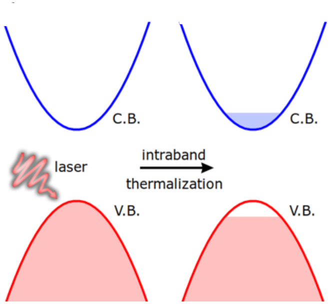


How to efficiently simulate phonon and structural dynamics at very long times ?

Constrained Density functional perturbation theory for photexcited insulators

Giovanni Marini and Matteo Calandra, Phys. Rev. B **104**, 144103 (2021)

- Complete cDFPT framework : two different chemical potentials and electron-hole plasma distribution, no supercells.



We build on top of Refs.:

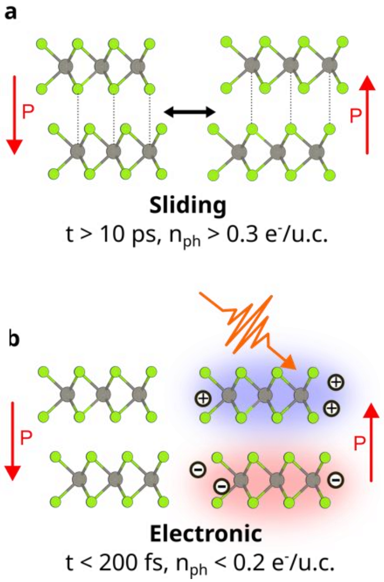
S. De Gironcoli, Phys. Rev. B 51, 6773(R) (1995)
Tangney & Fahy, PRL **82**, 4340 (1999), PRB Phys. Rev. B **65**, 054302 (2002)

- Complete structural optimization (forces/cell optimization).
- Vibrational properties (phonon dispersion)
- Electron-phonon interaction (including photocarriers-photocarriers screening)
- Coupling with SSCHA, Machine-learning based MD, *ab initio* BOMD, CPMD

A. Corradini, G. Marini and M.C., npj Computational Materials 11, 151 (2025)

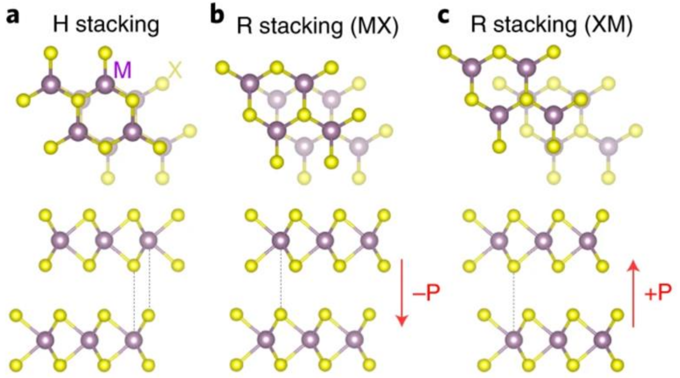
How does all this framework works ?

Light-Induced Transient Polarization Reversal in Rhombohedrally Stacked Bilayer Transition-Metal Dichalcogenides via an Electronic Mechanism



X. Zhou, S. Mocatti and M.C. https://arxiv.org/abs/2605.25982.

Polarization control in **rhombohedrally** stacked TMD bilayers



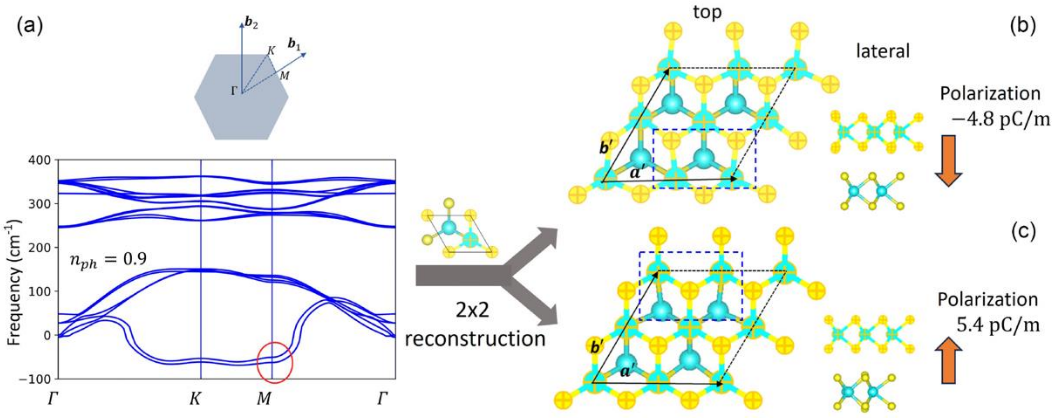
Wang *et al.* Nature Nanotechnology 17,367 (2022)

- Rhombohedrally stacked TMDs bilayers host an intrinsic polarization.
- Sliding one layer with respect to the other leads to a polarization inversion.
- Controlling the sliding is equivalent at controlling the polarization.

Controlling the polarization at the nanoscale is crucial for non-volatile and volatile ultrafast all-optical memories

Light-induced polarization switching in rhombohedrally stacked TMD bilayers

> 0.3 photoexcited carriers / unit cell

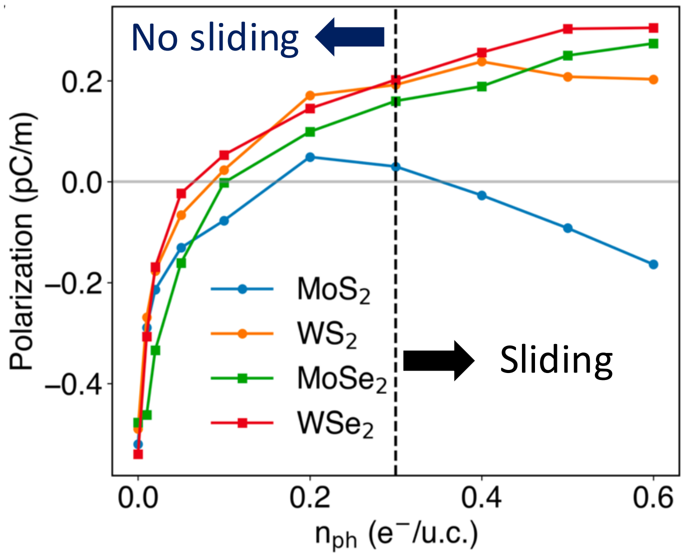


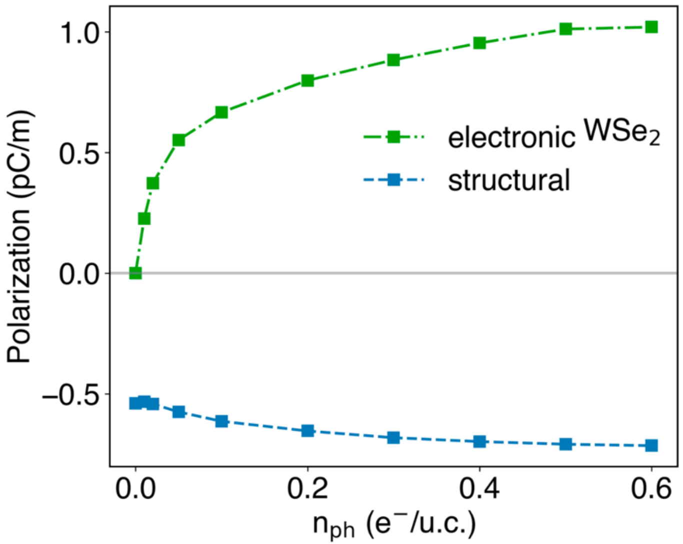
- It has been proposed that at very large fluences a structural sliding instability occurs

Q. Yang and S. Meng, Phys. Rev. Lett. 133, 136902 (2024).
L. Gao and L. Bellaiche, Phys. Rev. Lett. 133, 196801 (2024).

- However, at such large fluences it is easy to damage the sample.
  Moreover, the polarization switching occurs on the 10 ps timescale

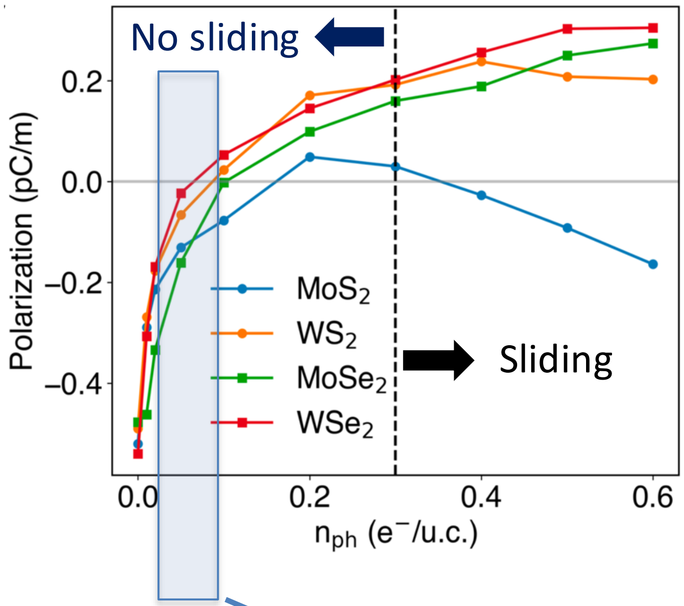
Ultrafast Light induced polarization inversion in rhombohedrally stacked TMD

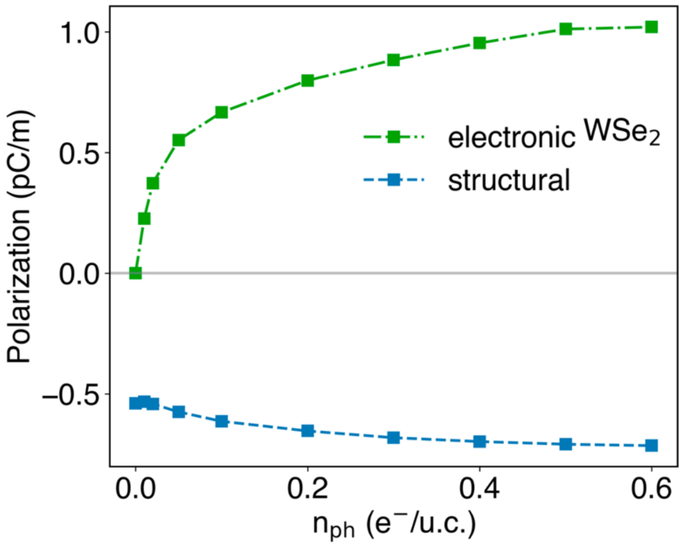




cDFPT calculations

Ultrafast Light induced polarization inversion in rhombohedrally stacked TMD





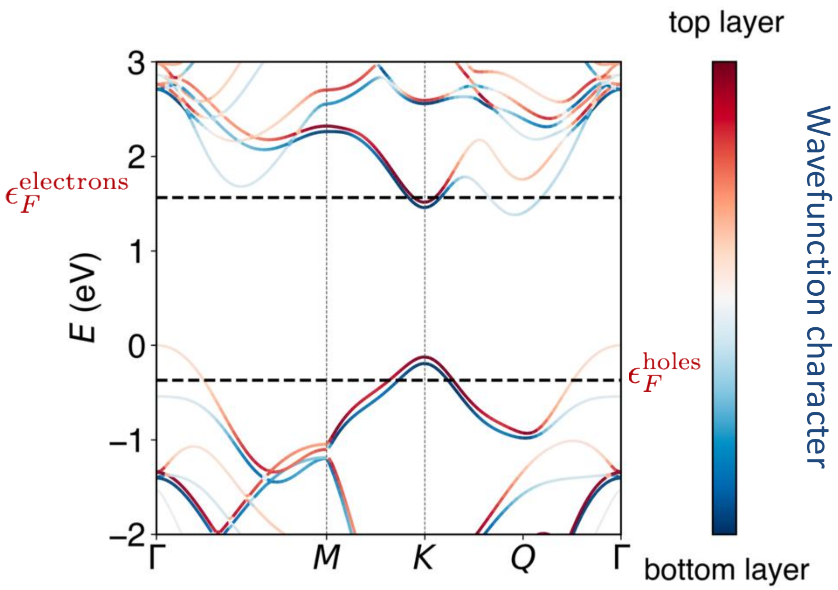
The polarization switching is completely electronic! NO SLIDING !

Why ? How ?

cDFPT calculations

Mechanism for ultrafast light switching of polarization

cDFT calculation



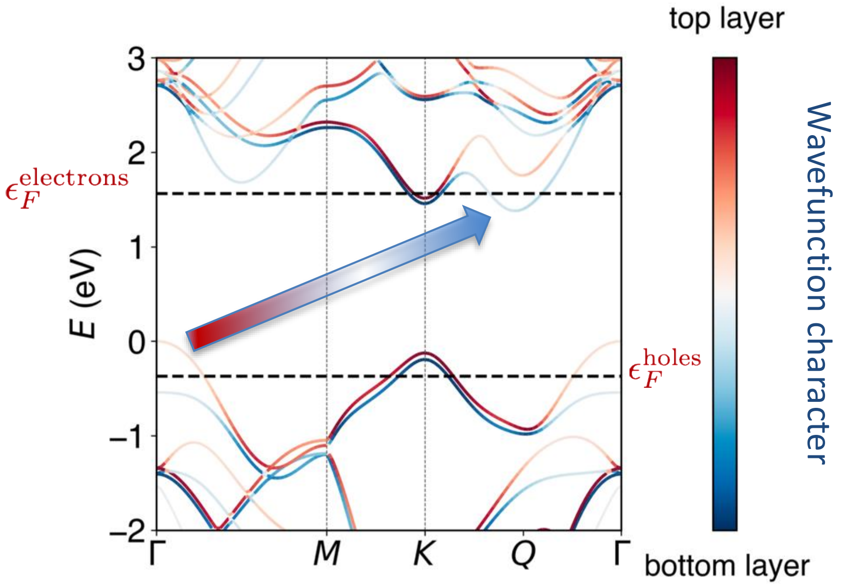
WSe2 R-bilayer

Band edges are localized on opposite layers (effective type II band alignement).

The thermalization of the photocarriers is an effective transfer of electrons from one layer to the other.

Mechanism for ultrafast light switching of polarization

cDFT calculation



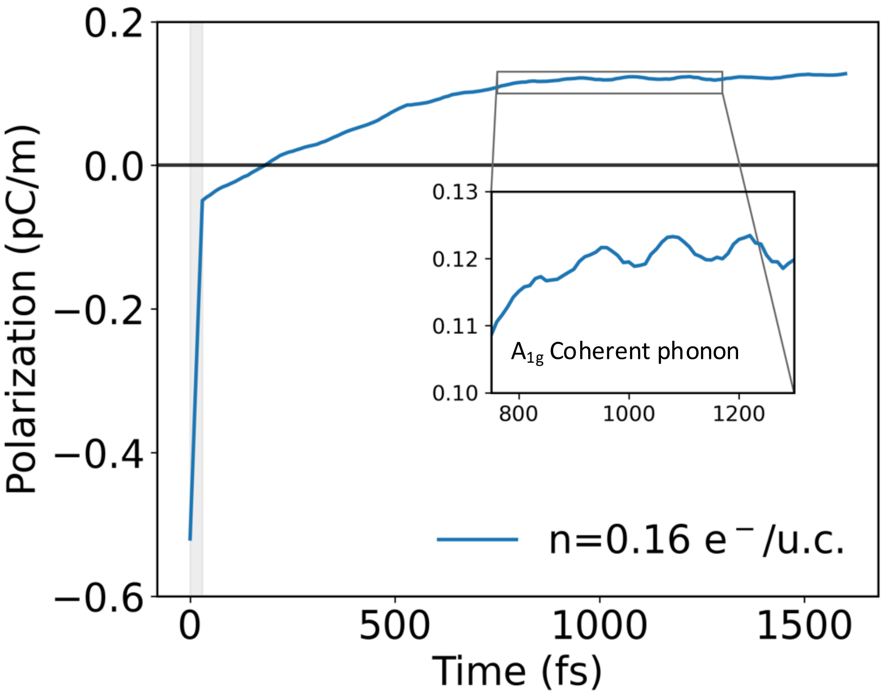
WSe2 R-bilayer

Band edges are localized on opposite layers (effective type II band alignement).

The thermalization of the photocarriers is an effective transfer of electrons from one layer to the other.
(and from Se states to W planar states)

How fast is the polarization switching ?

WSe2 R-bilayer

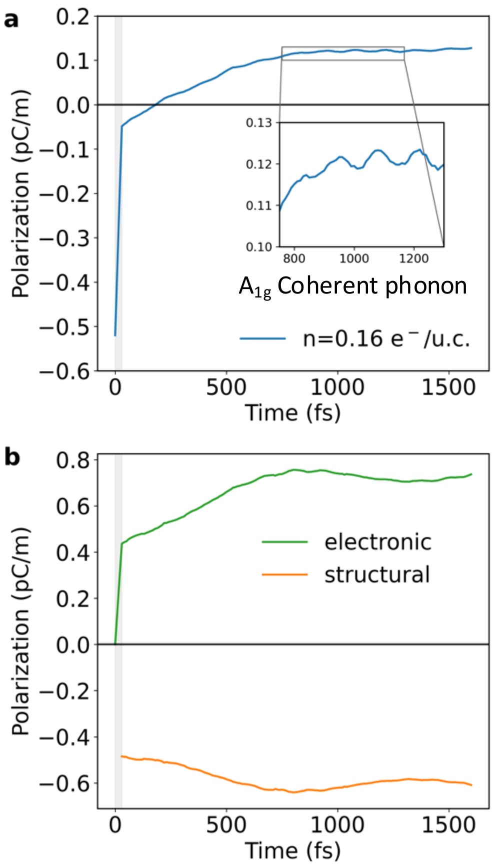


Complete manybody dynamics

Polarization switching in less than 200 fs, approximately 50 times faster than with sliding !

How fast is the polarization switching ?

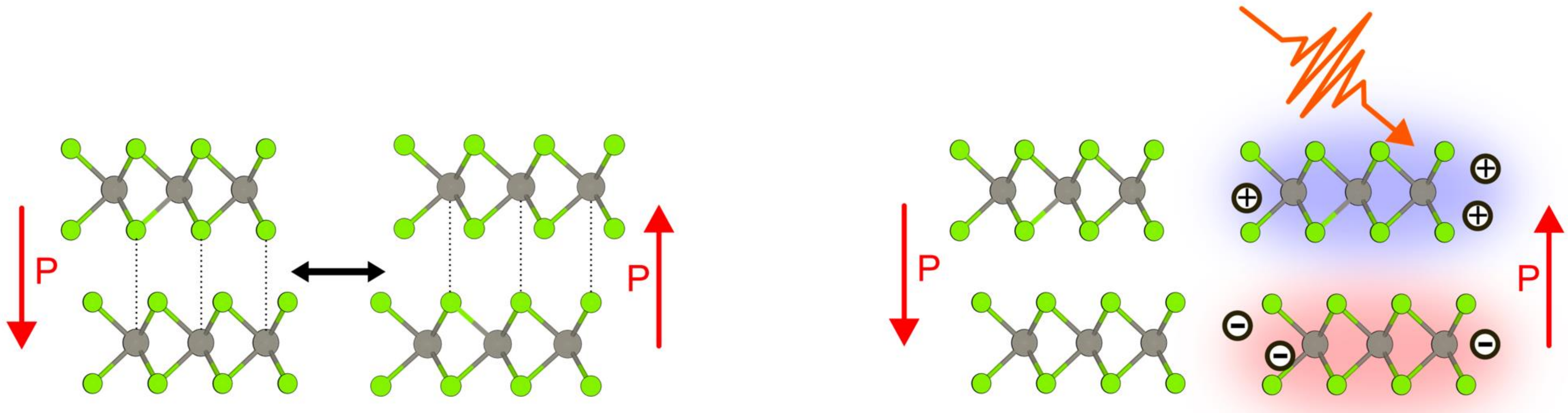
WSe2 R-bilayer



Complete manybody dynamics

Completely electronic effect!

Light-induced polarization switching in less than 200 fs, faster than ever !



Sliding

t > 10 ps, n_{ph} > 0.3 e^-/u.c.

Electronic

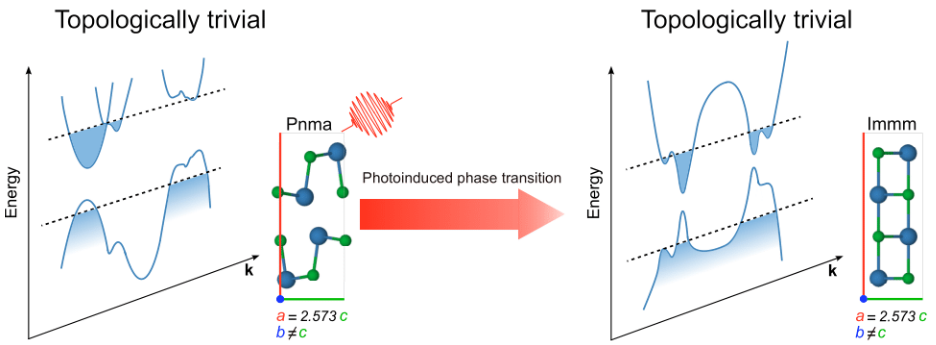
t < 200 fs, n_{ph} < 0.2 e^-/u.c.

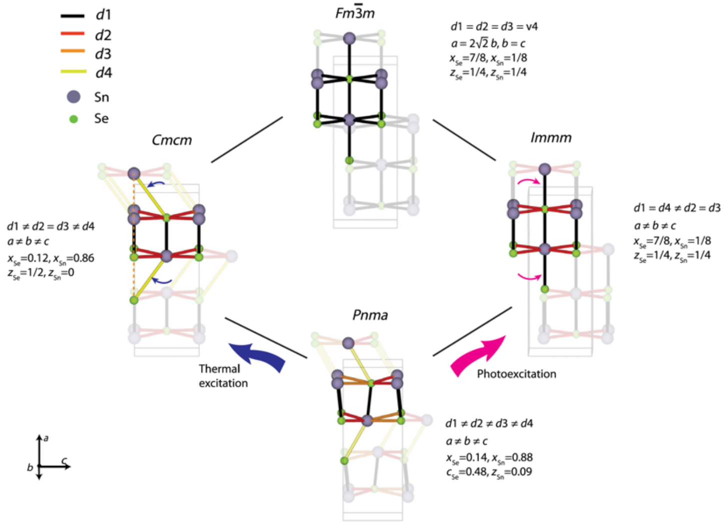
X. Zhou, S. Mocatti and M.C. https://arxiv.org/abs/2605.25982.

Photoexcited SnSe

S. Mocatti, G. Marini and M.C., J. Phys. Chem. Lett. **14**, 41, 9329 (2023)

Non-thermal pathway to the topologically crystalline insulator state in SnSe





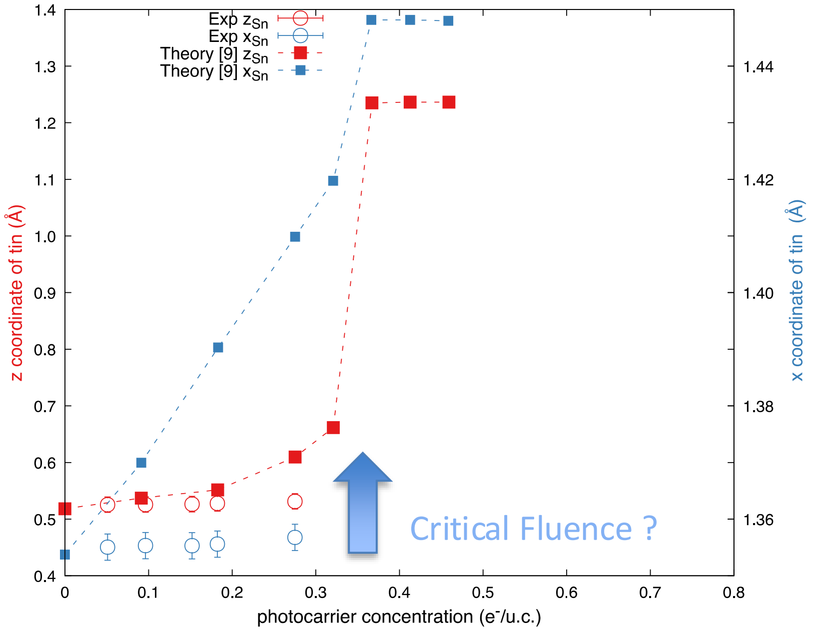
Huang *et al.* PRX 12, 011029

Thermal phase transition : Pnma → Cmcm (T_c=807 K)

Non-Thermal phase transition : Pnma → Imm ?

Critical fluence ? What happens after recombination ?

Ultrafst XRD in SnSe as a function of photocarrier concentration



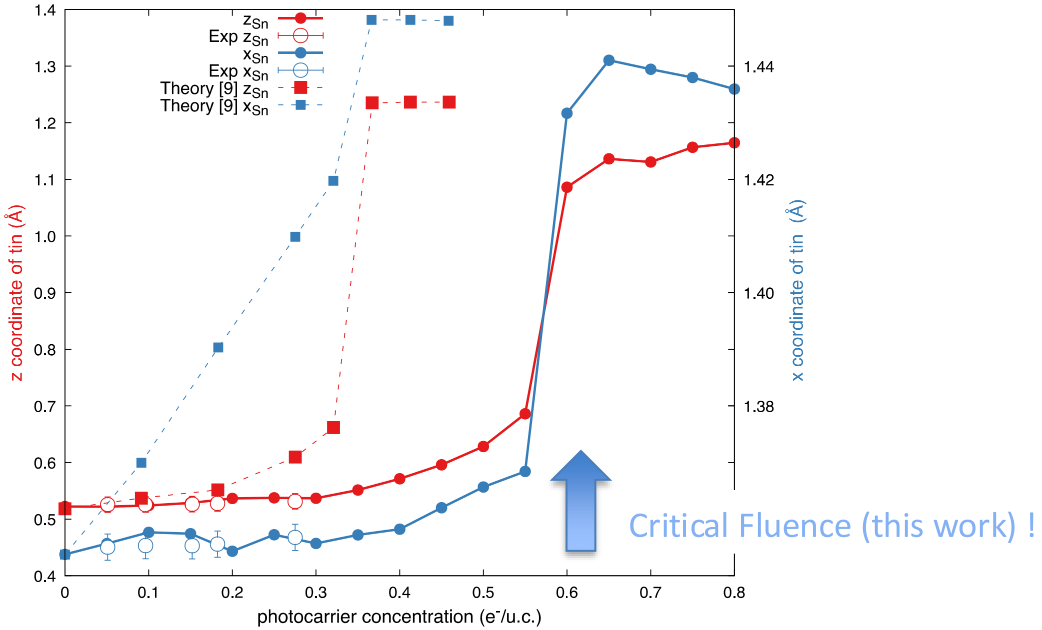
Huang *et al.* PRX 12, 011029

Strong disagreement Theory Experiment.

Incorrect estimate of the critical fluence for the transition.

Ultrafst XRD in SnSe as a function of photocarrier concentration

Huang *et al.* PRX 12, 011029 (2022)



Excellent agreement theory v.s. experiments when the electron-hole plasma is explicitely included.

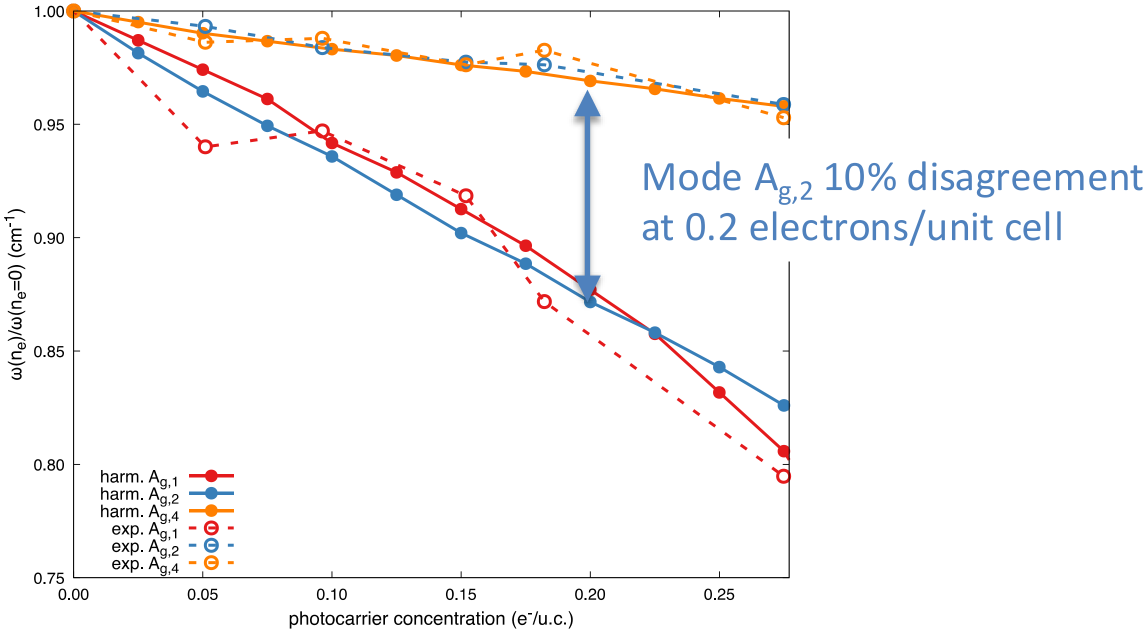
Experiments in Huang *et al.* still quite far from the critical fluence.

S. Mocatti, G. Marini and M.C., J. Phys. Chem. Lett. 14, 41, 9329 (2023)

G. Marini and M.C., PRB 104, 144103 (2021)

Displacive excitations coherent phonons in SnSe

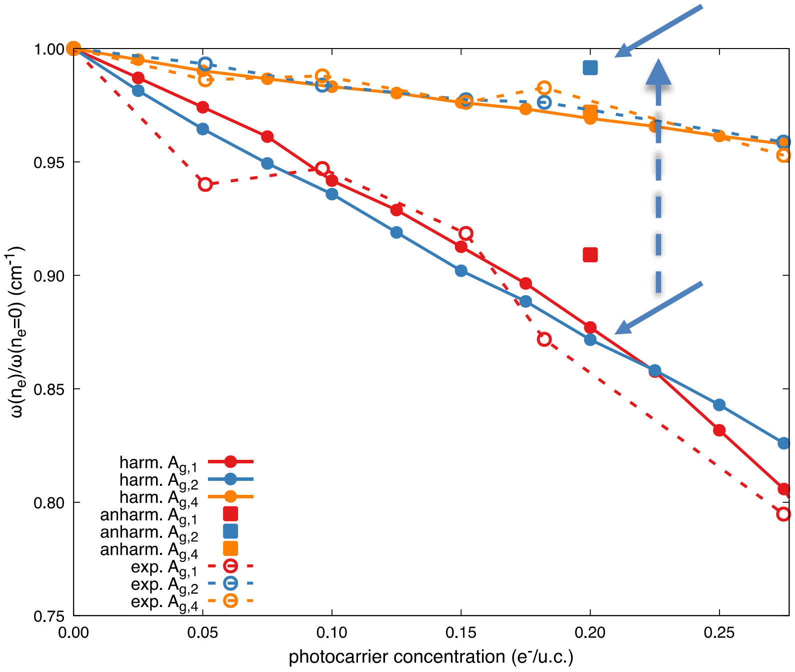
Huang *et al.* PRX 12, 011029 (2022)



Harmonic theory: excellent agreement except for mode $A_{g,2}$

S. Mocatti, G. Marini and M.C., J. Phys. Chem. Lett. 14, 41, 9329 (2023)

Displacive excitations coherent phonons in SnSe



Huang *et al.*
PRX 12, 011029

SSCHA
Stochastic Self-Consistent Harmonic Approximation

See L. Monacelli lectures

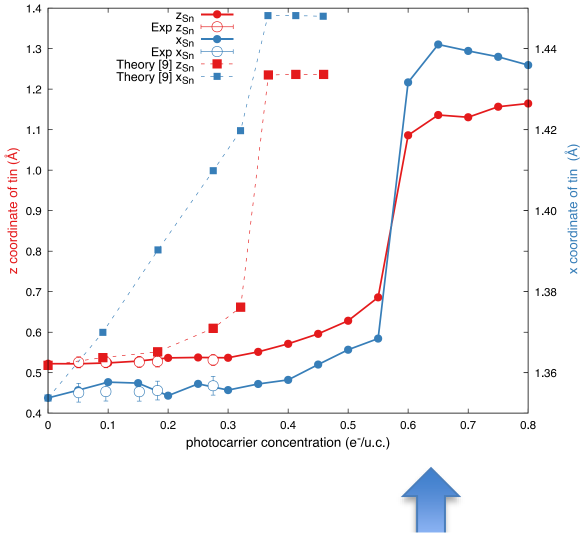
Crucial role of light-induced quantum anharmonicity !

Error on the quantun free energy curvature of the photoexcited state below 2% !

S. Mocatti, G. Marini and M.C., J. Phys. Chem. Lett. 14, 41, 9329 (2023)

New experiment with better heat dissipation spot on our prediction !

Predicted critical fluence
5 mJ/cm^2



Critical Fluence (this work) !

S. Mocatti, G. Marini and M.C.,
J. Phys. Chem. Lett. 14, 41, 9329 (2023)

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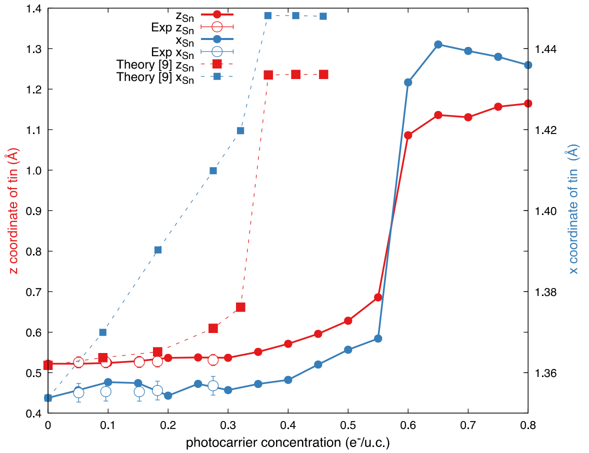
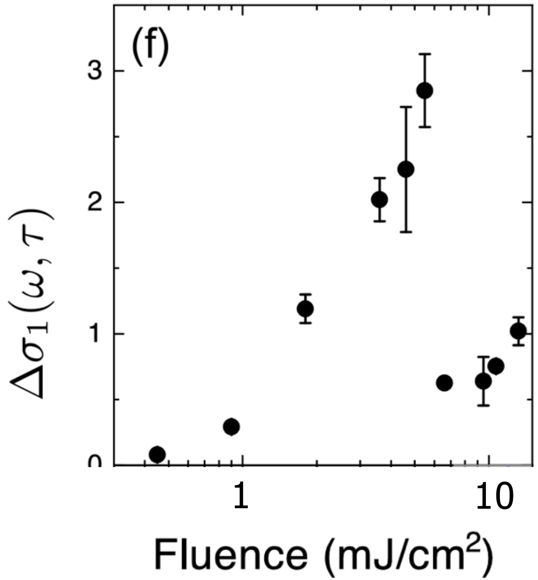


Critical Fluence (this work) !

S. Mocatti, G. Marini and M.C.,
J. Phys. Chem. Lett. 14, 41, 9329 (2023)

At 6 mJ/cm² sharp drop in THz differential conductivity



Dringoli *et al.*
PRL 132, 146901 (2024)

ω=10 THz, τ=1 ps

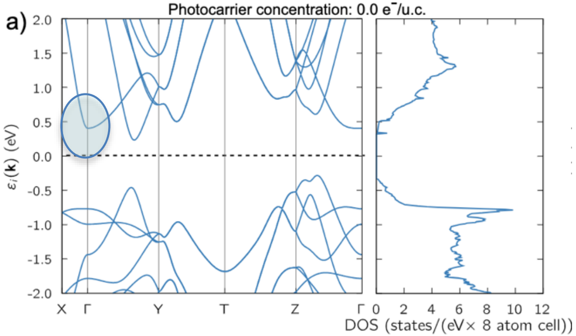
ONLY 1 mJ/cm² difference in critical fluence !

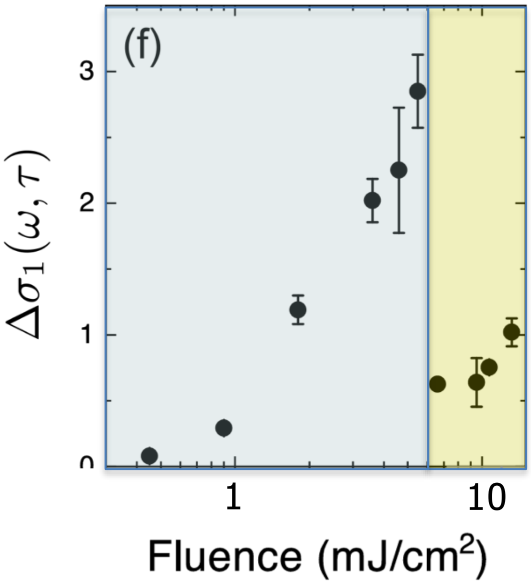
New experiment with better heat dissipation spot on our prediction !

1.55 eV excitation

At 6 mJ/cm^2 sharp drop in THz differential conductivity

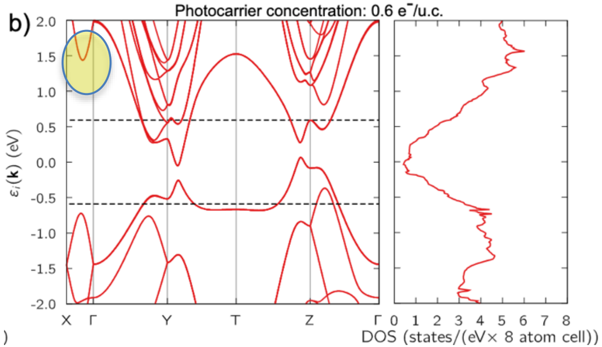
Pnma





ω=10 THz, τ=1 ps

Immm



$$\Delta\sigma_1(\omega,\tau)$$

Change in the electronic structure affects ThZ conductivity

S. Mocatti, G. Marini and M.C.,
J. Phys. Chem. Lett. 14, 41, 9329 (2023)

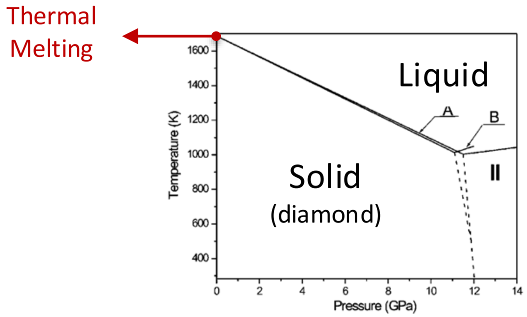
Dringoli *et al.*
PRL 132, 146901 (2024)

Scalable machine learning approach to light-induced order-disorder phase transitions with *ab initio* accuracy

A. Corradini, G. Marini and M. C., npj computational materials 11, 151 (2025)

Non-thermal melting in Si

- Thermal melting in silicon occurs in silicon slightly above 1600 K



Voronin *et al.* Phys. Rev. B 68, 020102 (2003).
A, B = data from different papers

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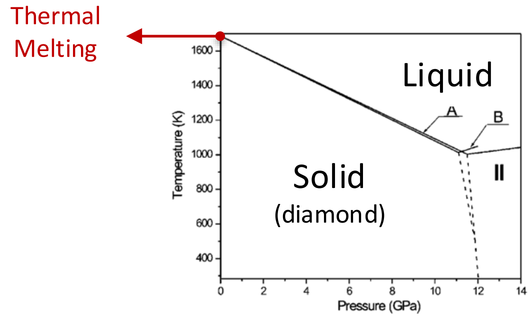

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- Non-thermal melting occurs at 0.2-0.4 photoexcited e^-/Si and at lower temperatures

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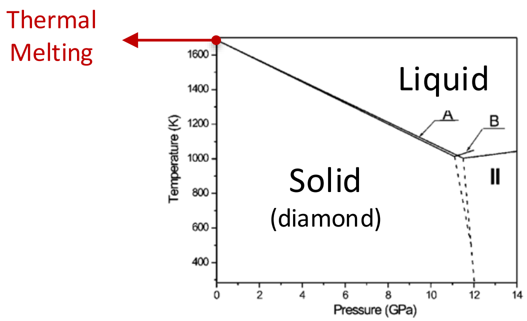


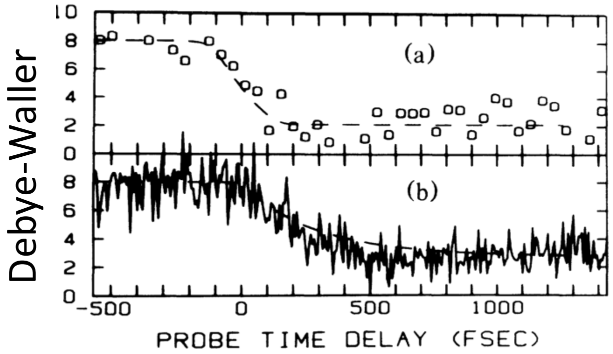
Voronin *et al.* Phys. Rev. B 68, 020102 (2003).
A, B = data from different papers

- Non-thermal melting occurs at 0.2-0.4 photoexcited e^-/Si and at lower temperatures.

- Non-thermal melting occurs on the hundreds fs and it is measured by drop in the Debye-Waller factor.

$$I(t) = I_0 \exp\left[-\frac{q^2 \mathrm{RMSD}(t)^2}{3}\right]$$

q=|**q**| = reciprocal lattice vector



Tom *et al.*, Phys. Rev. Lett. **60**, 1438 (1988).

Non-thermal melting in Si

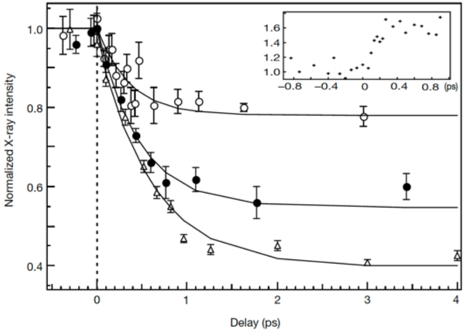
- Non-thermal melting of semiconductors still not understood:

  Is it a first or second order transition ?
  How does it occur ?

  1st order, Stampfli and Bennemann,
  Silvestrelli et al. Phys. Rev. Lett. **77**, 3149 (1996),
  2nd order, E. Zijlstra *et al.*, Phys. Rev. X 3, 011005 (2013).

Non-thermal melting in semiconductors measured at femtosecond resolution

A. Rousse*, C. Rischel†, S. Fourmaux*, I. Uschmann‡, S. Sebban*, G. Grillon*, Ph. Balcou*, E. Förster‡, J.P. Geindre§, P. Audebert§, J.C. Gauthier§ & D. Hulin*



Nature **410**, 65 (2001)

Non-thermal melting in Si

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  Silvestrelli et al. Phys. Rev. Lett. **77**, 3149 (1996),
  2nd order, E. Zijlstra *et al.*, Phys. Rev. X 3, 011005 (2013).

- Simulations of non-thermal melting suffer of two problems:

  MD uses non-physical very large Fermi temperature to simulate photoexcited carriers in quasi-equilibrium.

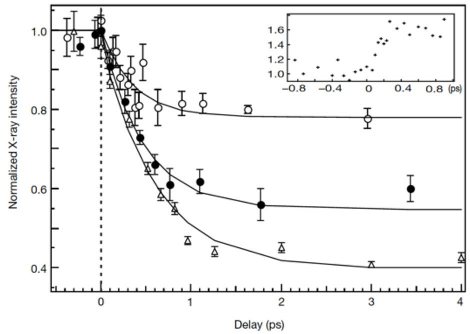
  Silvestrelli et al. Phys. Rev. Lett. **77**, 3149 (1996),
  Phys. Rev. B 56, 3806 (1997)

  TDDFT + Ehrenfrest small simulation boxes (< 256)
  non-size consistet results.

  W.-H. Liu *et al.*, Science Advances 8, eabn4430 (2022)

Non-thermal melting in semiconductors measured at femtosecond resolution

A. Rousse*, C. Rischel†, S. Fourmaux*, I. Uschmann‡, S. Sebban*, G. Grillon*, Ph. Balcou*, E. Förster‡, J.P. Geindre§, P. Audebert§, J.C. Gauthier§ & D. Hulin*



Nature **410**, 65 (2001)

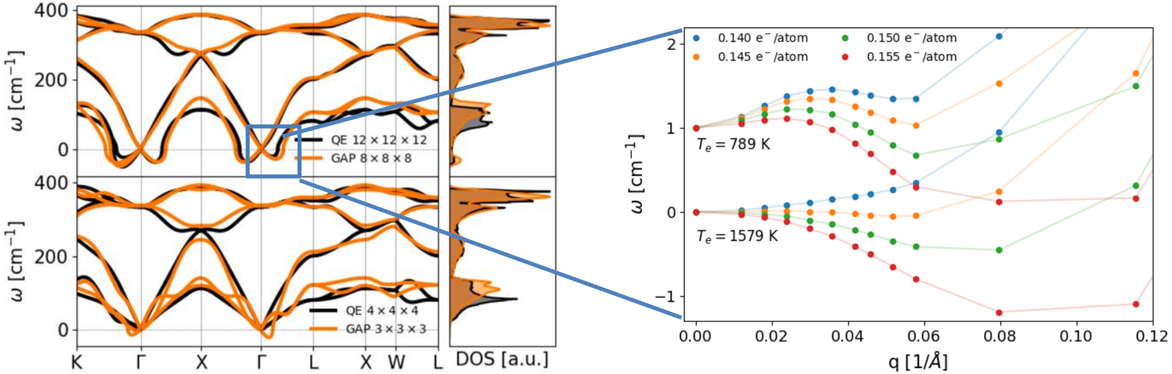
Our solution: NVE MD with machine learning potentials on top of cDFPT (two Fermi levels)

Machine Learning : Benchmarking

Photoexcited state

Ex. N_e=0.2 e^-/Si (28.2 mj/cm^2)

High Accuracy on phonon dispersion in the presence of the electron-hole plasma



Phonon instability invisible on small sim. boxes (< 216)

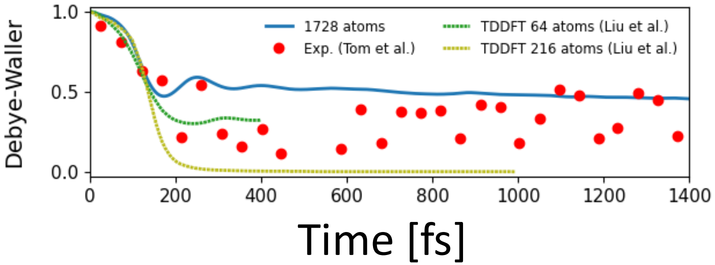
Phonons dynamically **unstable at N_e~ 0.2** (28.2 mJ/cm^2) with a **finite sound velocity (2nd order) !**

At larger fluences the sound velocity becomes negative.

MD simulations of non-thermal melting in the presence of an e-h plasma

Lattice temperature 300 K

N_e=0.2 e^-/Si



TDDFT+Ehrenfrest from
Liu *et al.* Science Advances 8, eabn4430 (2022)

MD simulations of non-thermal melting in the presence of an e-h plasma

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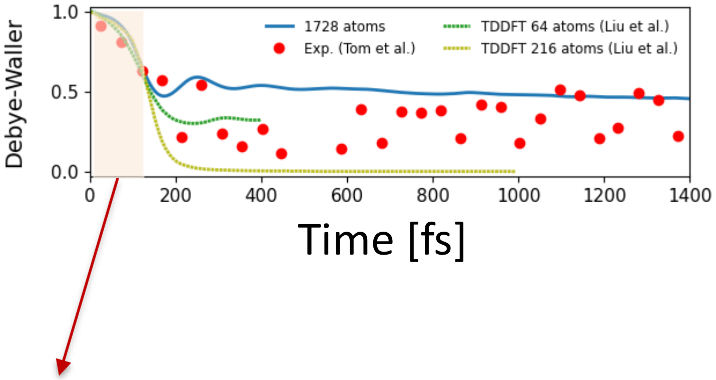


TDDFT+Ehrenfrest from
Liu *et al.* Science Advances 8, eabn4430 (2022)

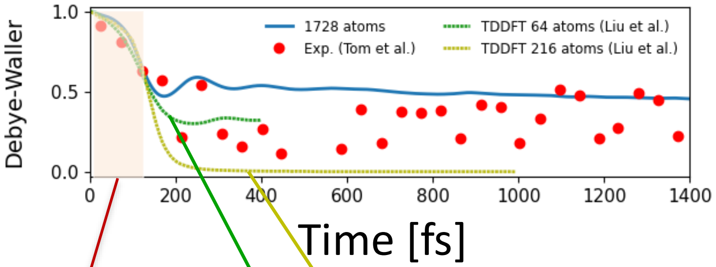
In the first 150 fs, TDDFT (Ehrenfrest) and MD ionic dynamics are practically identical !

Simulating ionic dynamics with « quasi-equilibrium » electrons is, once more, an excellent aproximation.

MD simulations of non-thermal melting in the presence of an e-h plasma

Lattice temperature 300 K

N_e=0.2 e^-/Si



TDDFT+Ehrenfrest from
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In the first 150 fs, TDDFT (Ehrenfrest) and MD ionic dynamics are practically identical !

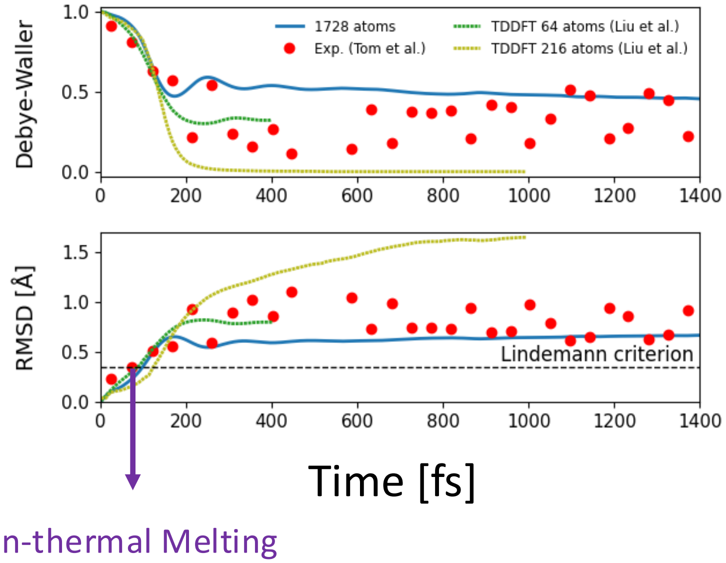
Simulating ionic dynamics with « quasi-equilibrium » electrons is, once more, an excellent aproximation.

At larger time TDDFT+Ehrenfrest results are different on 64 and 216 simulation boxes (no size consistency)!

MD simulations of non-thermal melting in the presence of an e-h plasma

Lattice temperature 300 K

N_e=0.2 e^-/Si



TDDFT+Ehrenfrest from
Liu *et al.* Science Advances 8, eabn4430 (2022)

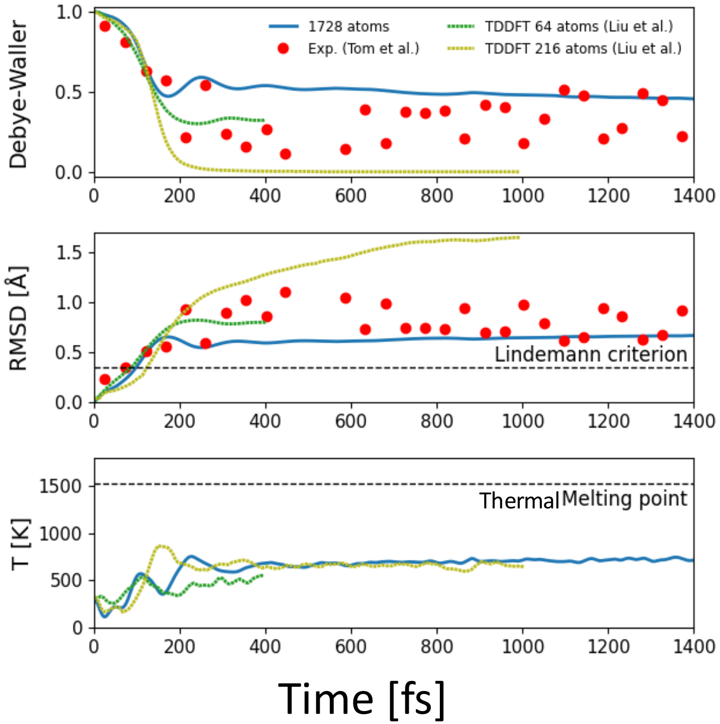
From the RMSD we see that the Si melt non thermally in less than 200 fs.

After it melts, TDDFT+Ehrenfrest breaks down, while MD in the quasi equilibrium e-h plasma approx. remains perfect (despite frozen electrons).

MD simulations of non-thermal melting in the presence of an e-h plasma

Lattice temperature 300 K

N_e=0.2 e^-/Si



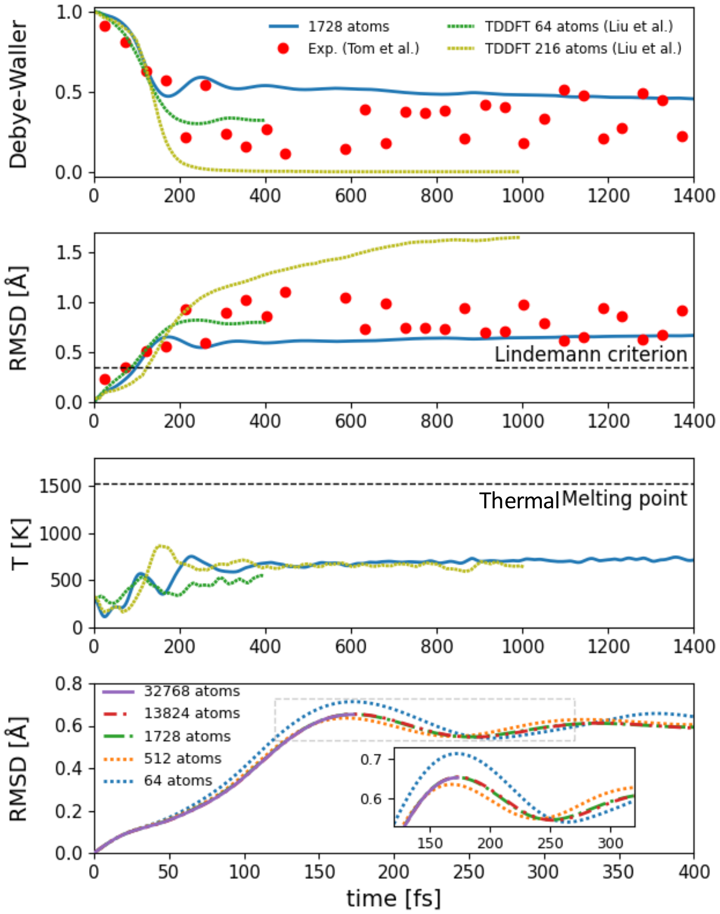
TDDFT+Ehrenfrest from
Liu *et al.* Science Advances 8, eabn4430 (2022)

The lattice temperature remains low (750 K<< thermal melting temperature) despite the Silicon melting.

MD simulations of non-thermal melting in the presence of an e-h plasma

Lattice temperature 300 K

N_e=0.2 e^-/Si

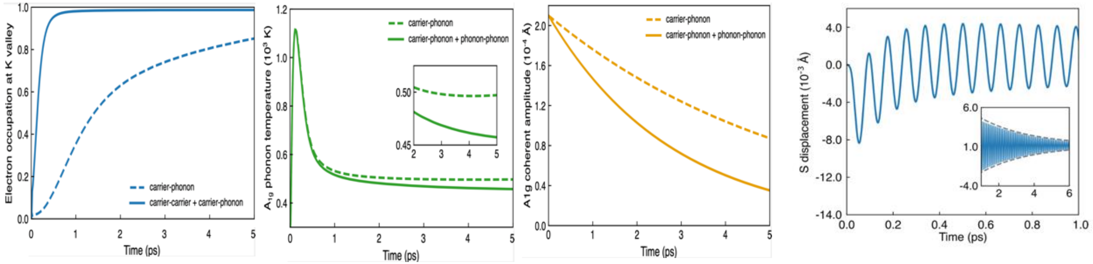


TDDFT+Ehrenfrest from
Liu *et al.* Science Advances 8, eabn4430 (2022)

No qualitative differences
up to 32768 atoms

Conclusions (1) - Methods

- Manybody out of equilibrium photocarriers and phonon dynamics including all scattering mechanisms from first principles.

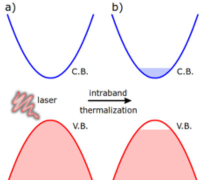


S. Mocatti *et al.* npj comp. Materials (2026)
10.1038/s41524-026-02104-y

https://the-epiq-team.gitlab.io/epiq-site/

- Constrained DFPT implementation available on Quantum Espresso Versions 7.4 or 7.5NC (developers).

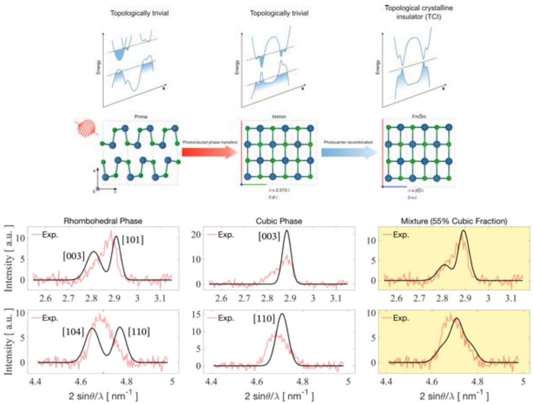
Giovanni Marini and MC, Phys. Rev. B **104**, 144103 (2021)



Hands on at 17h30 today

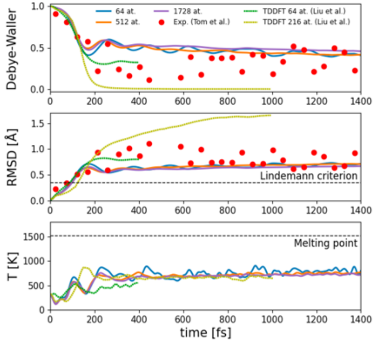
Conclusion (2) – Light induced phases in quantum materials

Photoexcited phase transitions in SnSe and GeTe.



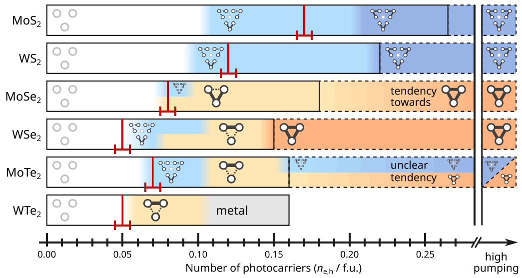
S. Mocatti, G. Marini and M.C., J. Phys. Chem. Lett. 14, 41, 9329 (2023).
M. Furci, G. Marini and M.C. , Phys. Rev. Lett. 132, 236101 (2024)

Non-thermal melting in solids (MD with ML potentials fitted on cDFPT).



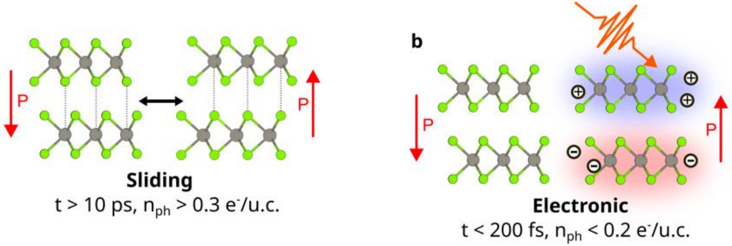
A. Corradini, G. Marini and M.C., npj Computational Materials 11, 151 (2025)

Light induced polaronic crystalline states in TMD single layers



G. Marini and M.C., PRL 127, 257401 (2021)
K. Holtgrewe, G. Marini and M. C., Nano Lett. 24, 13179 (2024)

Ultrafast polarization inversion in rhombohedrally stacked dichalcogenides bilayers.



X. Zhou, S. Mocatti and M.C. https://arxiv.org/abs/2605.25982.