Monte Carlo study of velocity fluctuations during transient regimes in monolayer graphene

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CAMPUS DE EXCELENCIA INTERNACIONAL

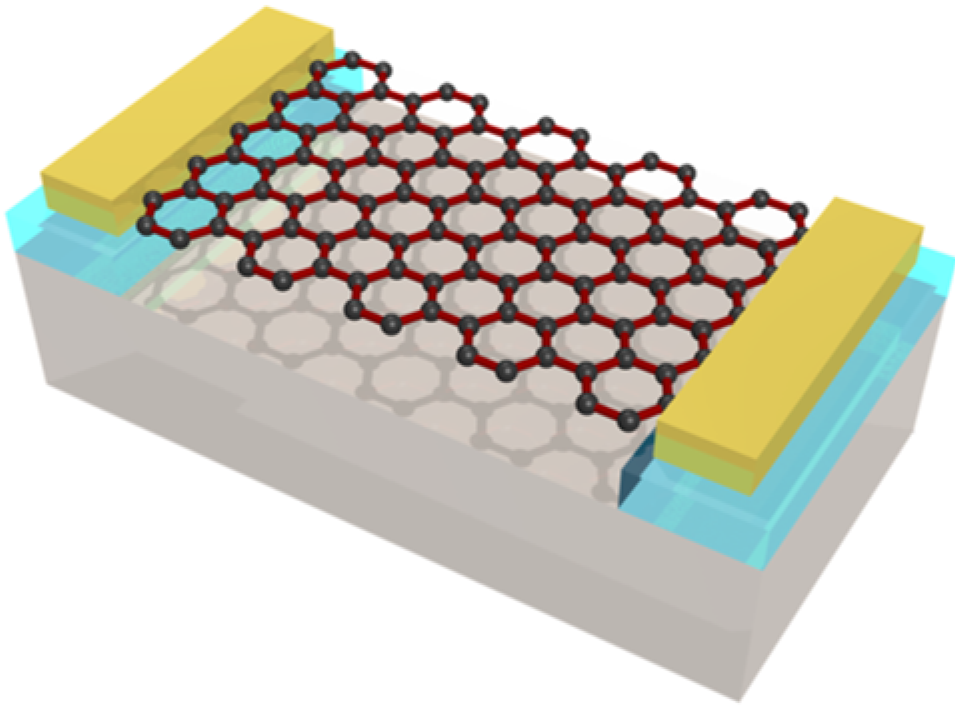
Outline

1. Introduction
   - Ensemble Material Monte Carlo model
   - Study of the transient velocity fluctuations
2. Results
   - Graphene on SiO2
     - Evolution of v, k, and ε
     - Low-to-high and high-to-low field: Tr. ACF and Tr. PSD
   - Comparison with other cases
3. Conclusions

1 Introduction

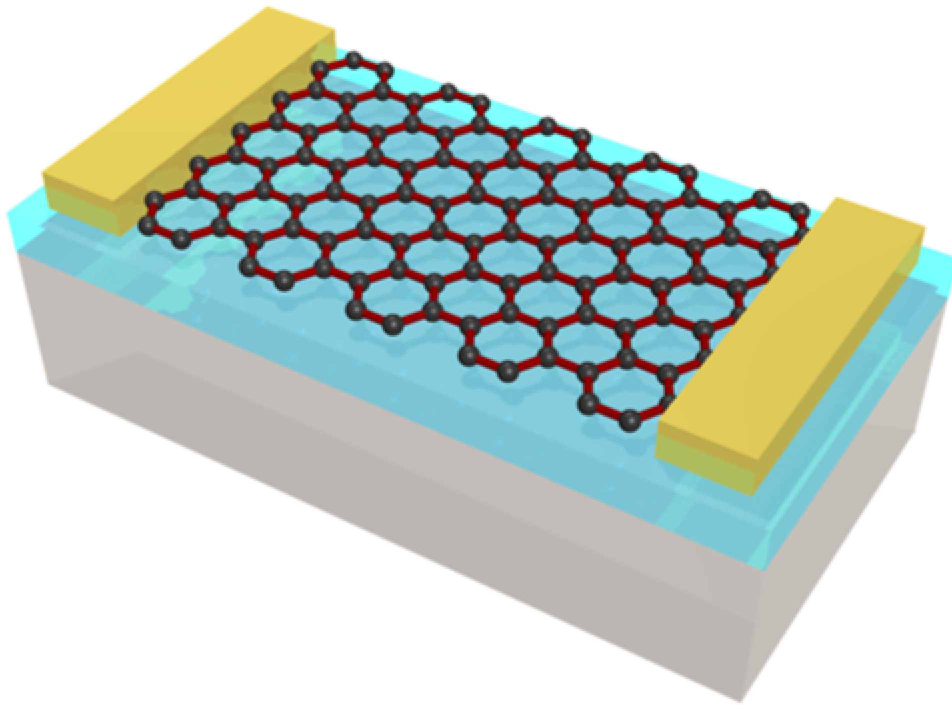
Why graphene?

- **Suspended graphene**:



  - Excellent electronic transport properties
  - Extremely high mobility at room temperature

- **Graphene on a substrate**



  - Typical substrates: SiO_2, h-BN, SiC, HfO_2, etc.
  - Transport properties affected by scattering with substrate phonons (SPPs), impurities, lattice defects…

Ensemble Material Monte Carlo model

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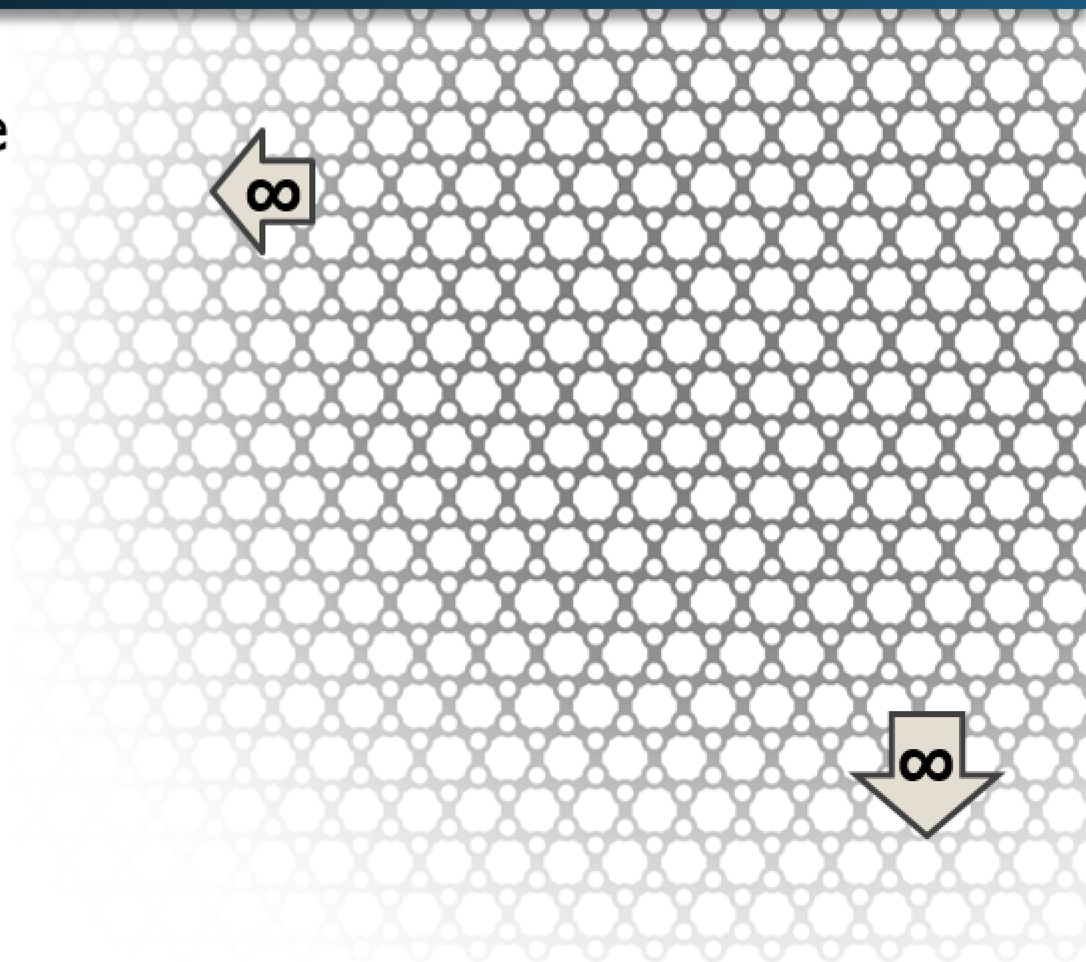

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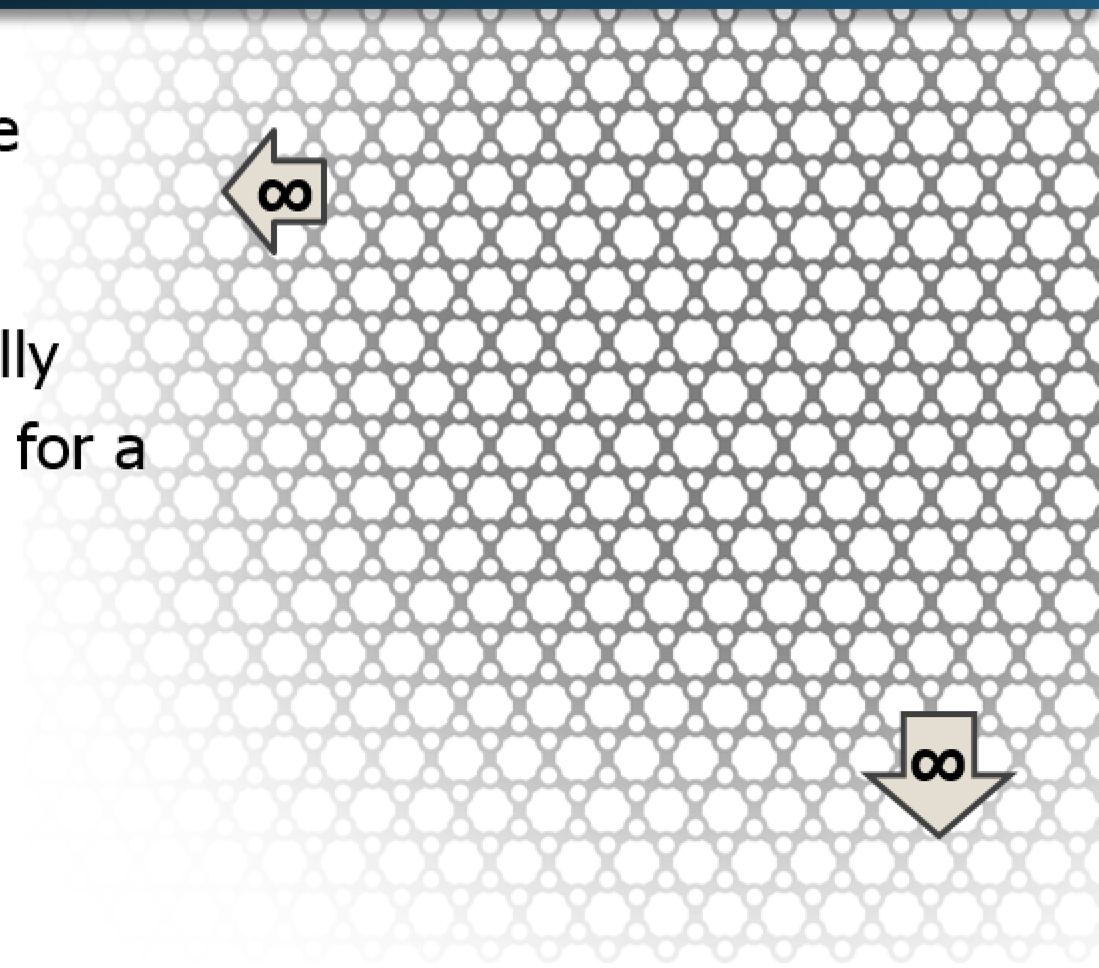
2. An **ensemble** of "**superparticles**" (tipically 100000) is simulated in a gridded ***k*-space** for a given time step.



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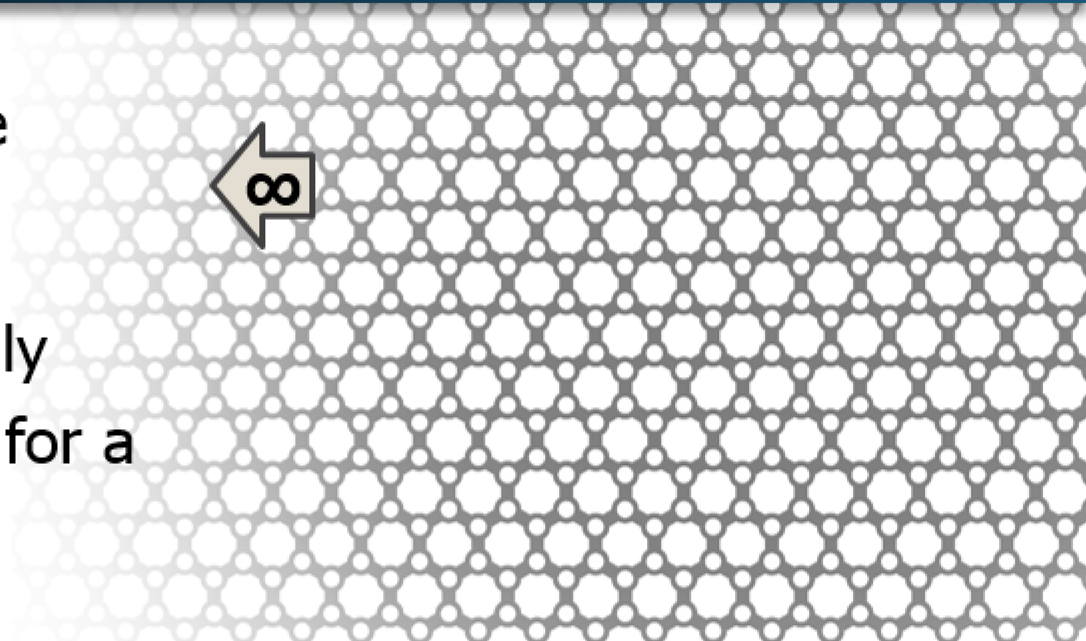

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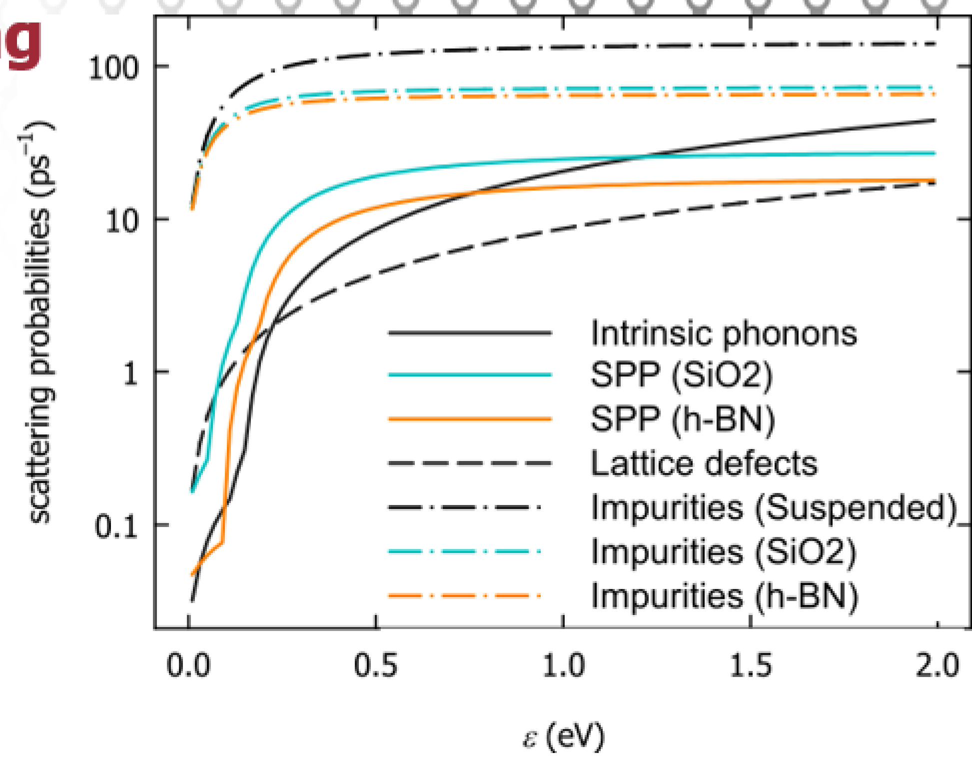

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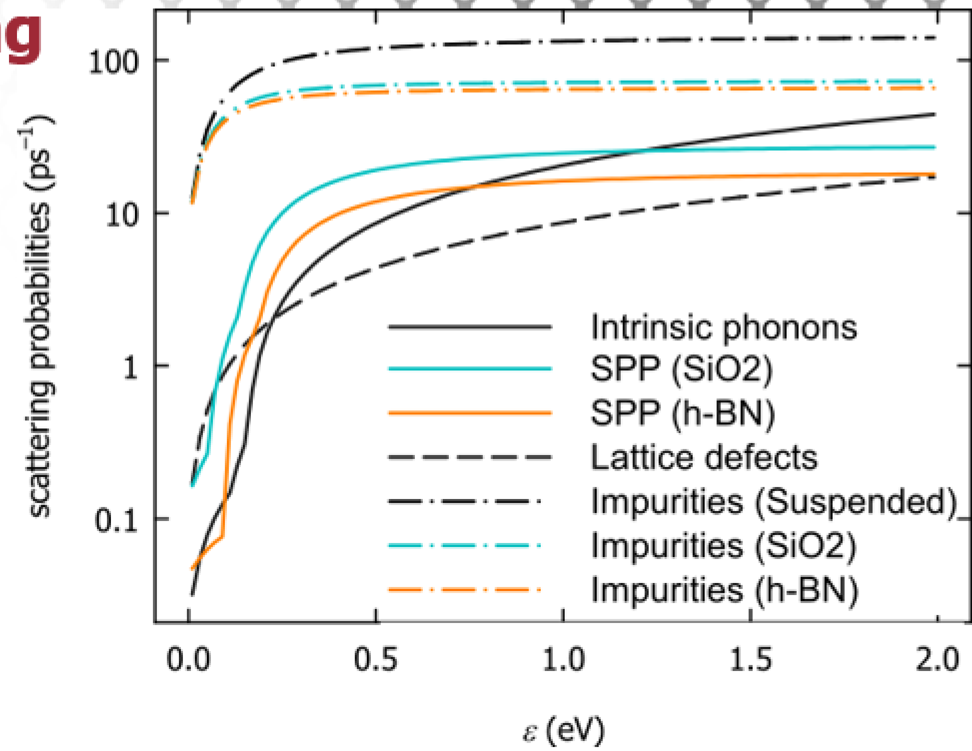
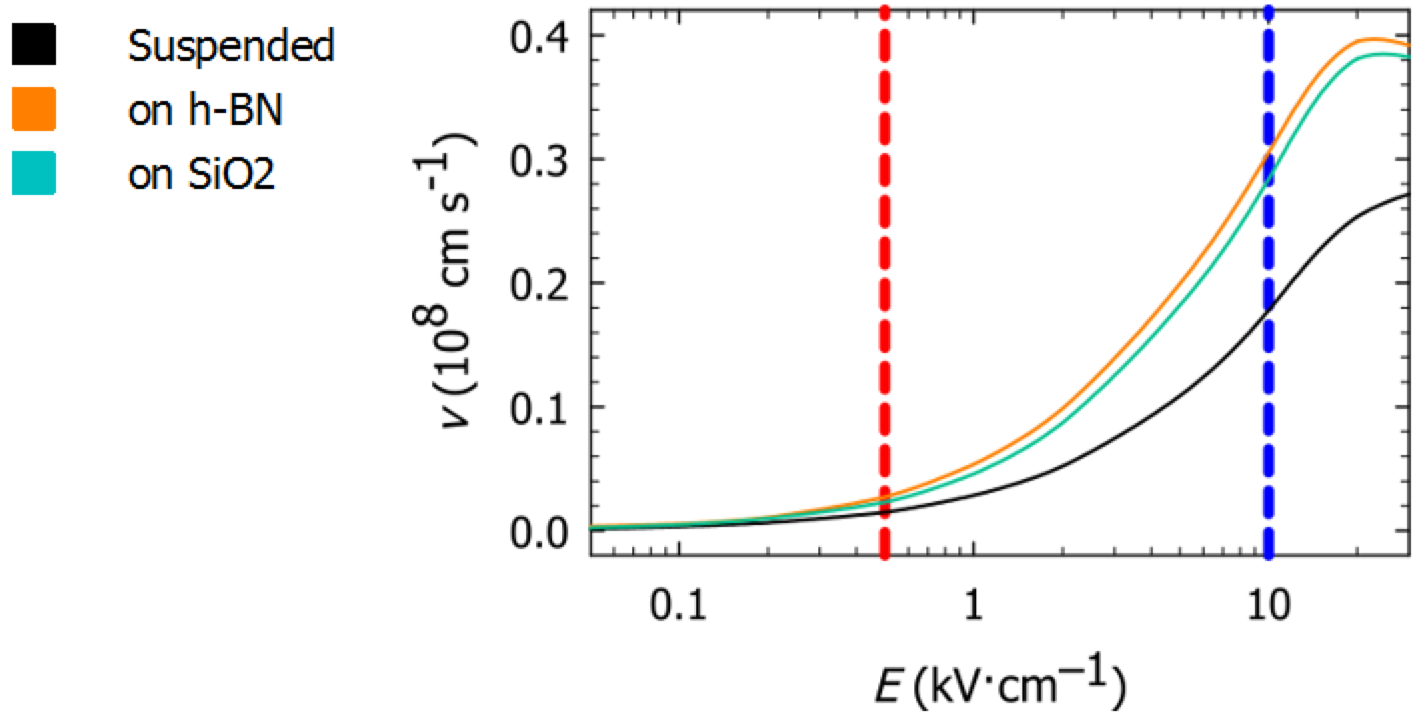
   and the **Pauli Exclusion principle**



Transient regimes for velocity fluctuations: High and low electrostatic field



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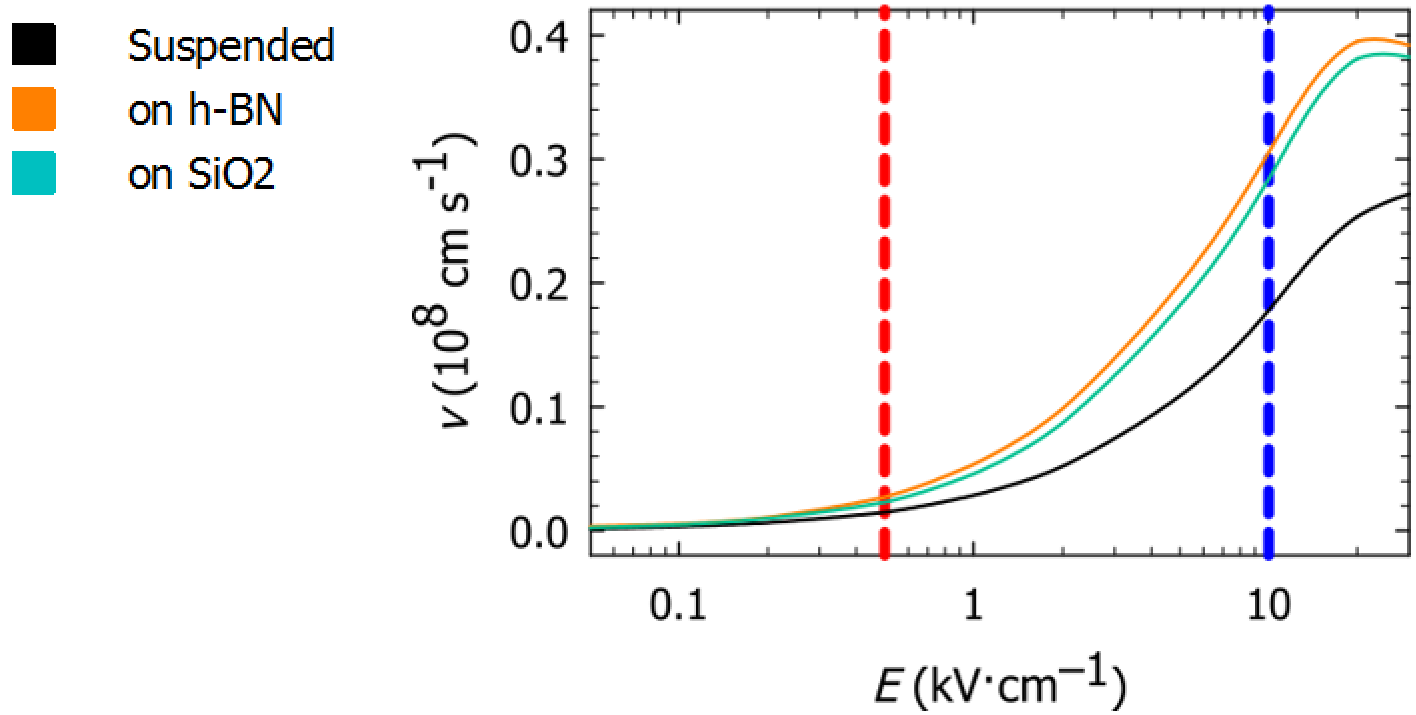

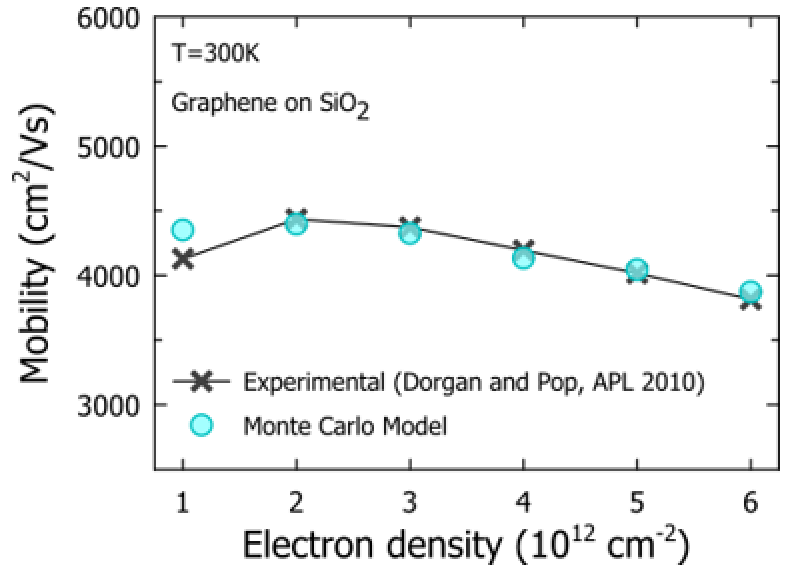

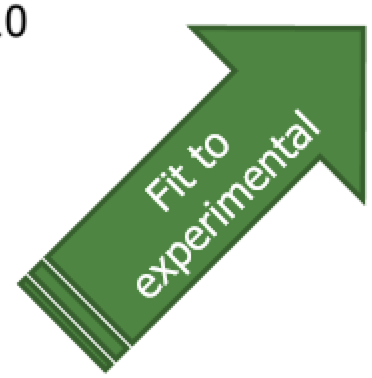

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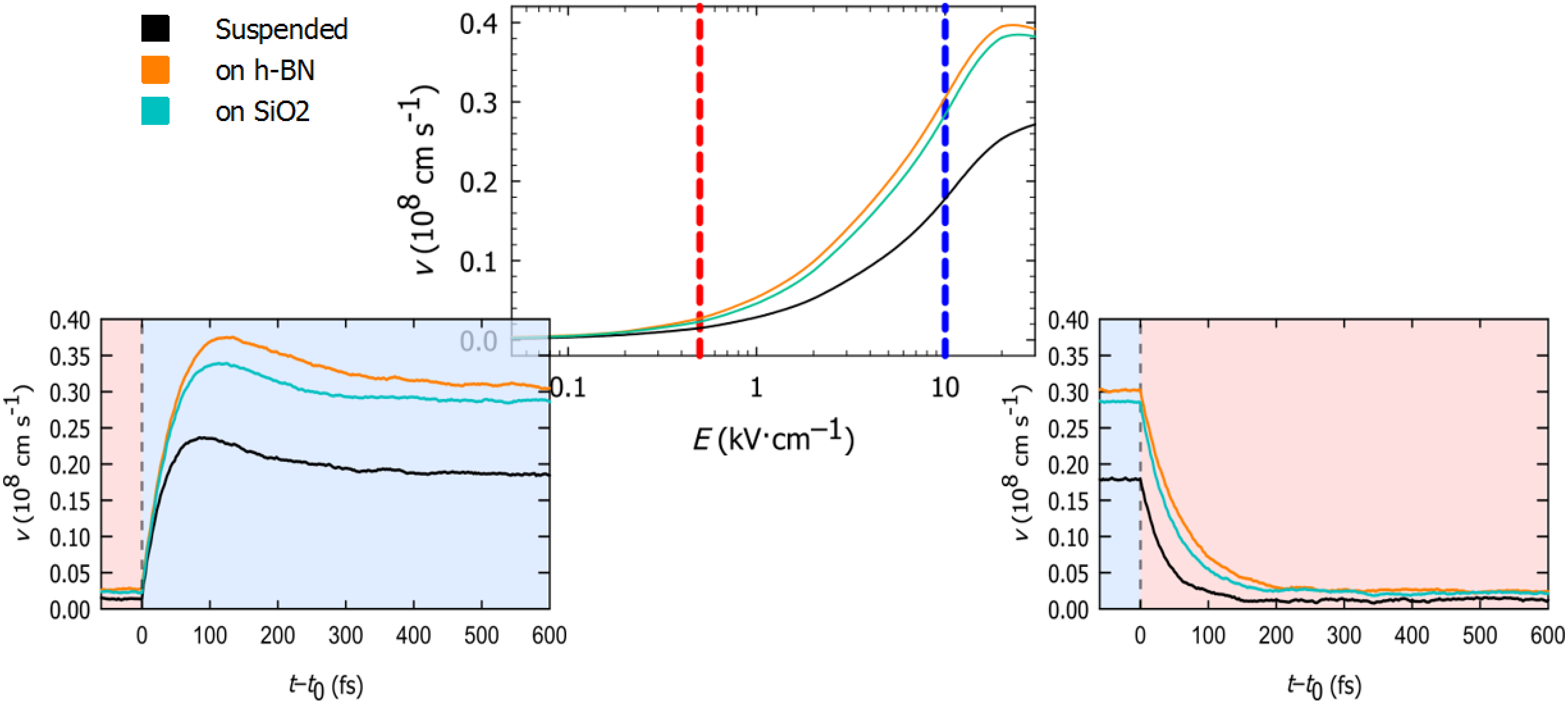

Low→high field

High→low field

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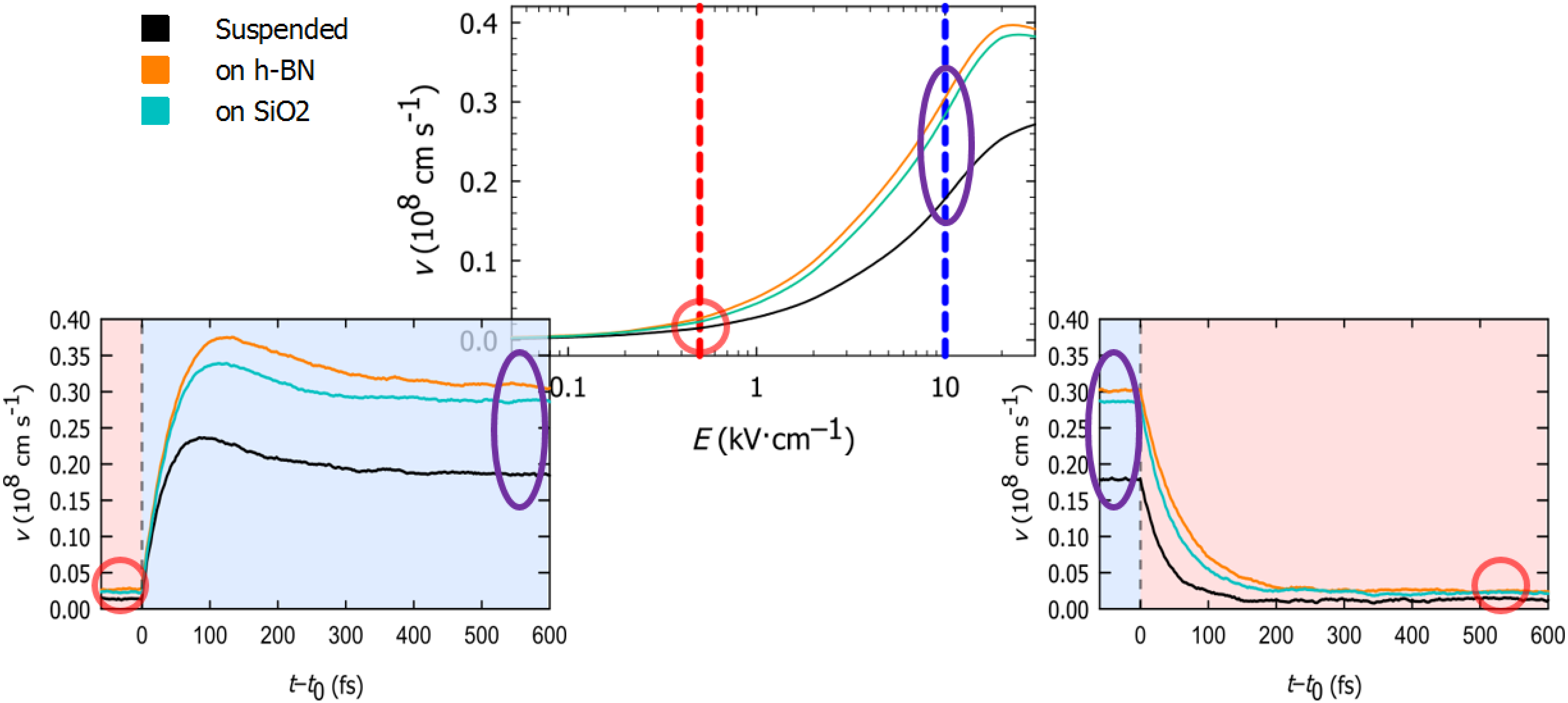

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Calculation of the Transient Autocorrelation Function

- Velocity fluctuations in a transient

$$\delta v(t) = v(t) - v_d(t) = v(t) - \langle v(t) \rangle$$

$$\langle \xi \rangle = \sum_{i=1}^{N} \frac{\xi_i}{N}$$

- Transient Autocorrelation Function

$$C_{\delta v}(t, \tau) = \langle \delta v(t) \delta v(t - \tau) \rangle$$

- Two-time correlation: τ, t:
extends towards the past: $t_0 \leq \tau \leq t$

[1] R. Brunetti, C. Jacoboni. *Phys. Rev. B* **29**, 5739 (1984)

Calculation of the Transient Autocorrelation Function

- The values of $\delta v(t)$ are stored at fixed times (Δt) for every superparticle in the ensemble:

	$t = 0 = t_0$	$t = \Delta t$	$t = 2\Delta t$	$\cdots$	$t = (n\text{-}1)\Delta t$	$t = n\Delta t$
1	$\delta v_{\mathbf{1}}(\,0\,)$	$\delta v_{\mathbf{1}}(\Delta t)$	$v_{\mathbf{1}}(2\Delta t)$	$\cdots$	$\delta v_{\mathbf{1}}((n\text{-}1)\Delta t)$	$\delta v_{\mathbf{1}}(n\Delta t)$
2	$\delta v_{\mathbf{2}}(\,0\,)$	$\delta v_{\mathbf{2}}(\Delta t)$	$\delta v_{\mathbf{2}}(2\Delta t)$	$\cdots$	$\delta v_{\mathbf{2}}((n\text{-}1)\Delta t)$	$\delta v_{\mathbf{2}}(n\Delta t)$
$\vdots$	$\cdots$	$\cdots$	$\cdots$	$\ddots$	$\cdots$	$\cdots$
N_p	$\delta v_{\mathbf{N_p}}(\,0\,)$	$\delta v_{\mathbf{N_p}}(\Delta t)$	$\delta v_{\mathbf{N_p}}(2\Delta t)$	$\cdots$	$\delta v_{\mathbf{N_p}}((n\text{-}1)\Delta t)$	$\delta v_{\mathbf{N_p}}(n\Delta t)$

$$C_{\delta v}(t,\tau) = \langle \delta v(t)\delta v(t-\tau)\rangle \qquad t_0 \le \tau \le t$$

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Contributions to the Autocorrelation Function

The contributions to $\delta v(t)$

$$\delta v(t) = \delta v_{\varepsilon}(t) + \delta v_{\mathbf{k}}(t)$$

Convective:	$\delta v_{\varepsilon}(t) = v_{\varepsilon}(t) - v_{d}(t)$
Thermal:	$\delta v_{\mathbf{k}}(t) = v(t) - v_{\varepsilon}(t)$

$$\begin{bmatrix} C_{\delta v,\varepsilon\varepsilon} & C_{\delta v,\varepsilon\mathbf{k}} \\ C_{\delta v,\mathbf{k}\varepsilon} & C_{\delta v,\mathbf{kk}} \end{bmatrix} = \begin{bmatrix} \langle \delta_{\varepsilon}(t)\delta_{\varepsilon}(t-\tau)\rangle & \langle \delta_{\varepsilon}(t)\delta_{\mathbf{k}}(t-\tau)\rangle \\ \langle \delta_{\mathbf{k}}(t)\delta_{\varepsilon}(t-\tau)\rangle & \langle \delta_{\mathbf{k}}(t)\delta_{\mathbf{k}}(t-\tau)\rangle \end{bmatrix}$$

[2] R. Brunetti, C. Jacoboni. *Phys. Rev. Lett.* **50**, 1164 (1983)

Calculation of the Transient Power Spectral Density

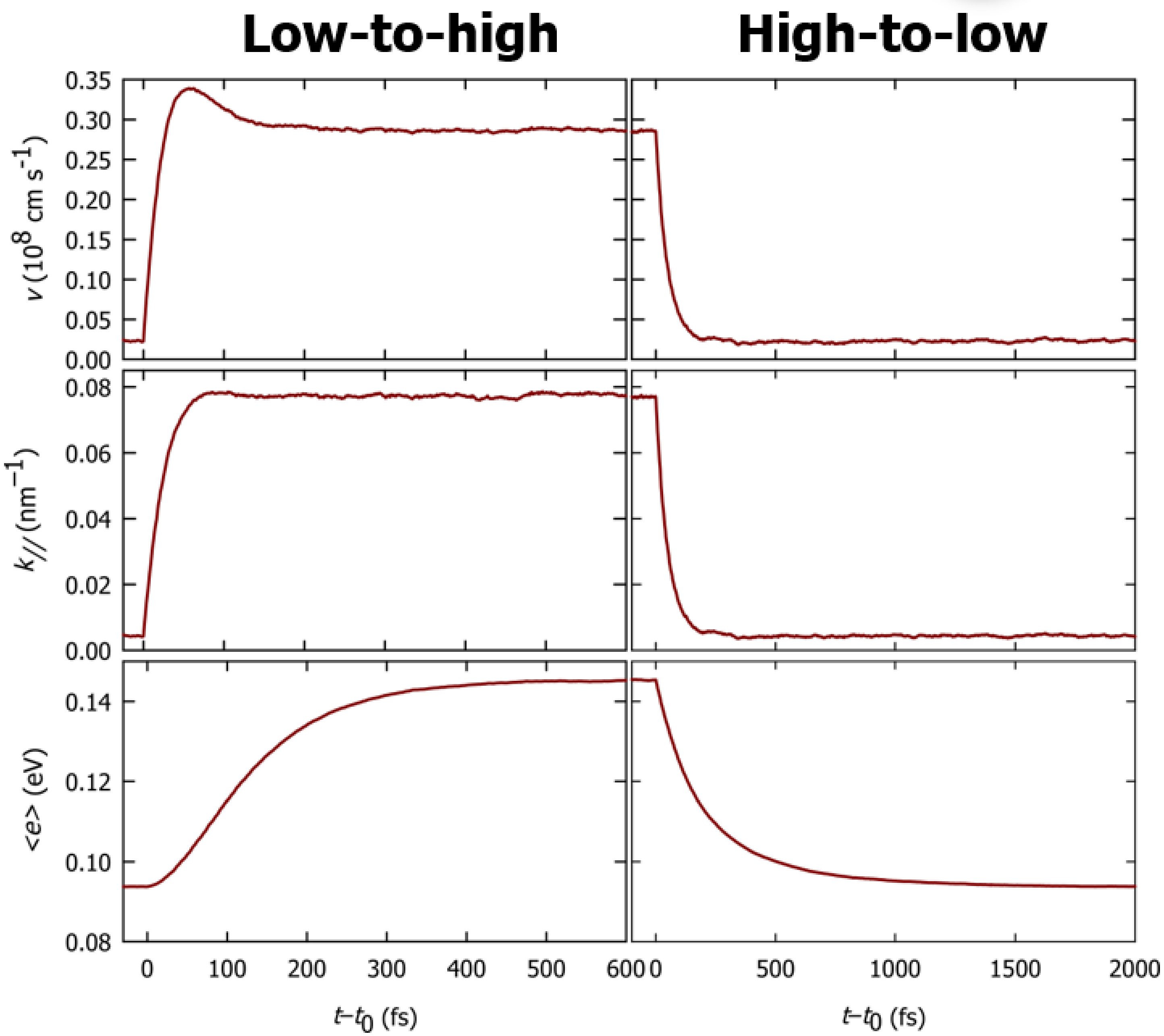
- $S_{\delta v}(f, \tau)$ provides the power dissipated **between t_0 and τ** during the transient for a frequency between f and f+df

$$S_{\delta v}(f,\tau) = \frac{1}{\tau}\left\langle \left| \int_{t_0}^{t} \delta v(t) \exp(j\omega t) \mathrm{d}t \right|^2 \right\rangle$$

[3] T. González, J. E. Velázquez et al. *Appl. Phys. Lett.* **60** 613 (1992)

3 Results

Graphene on SiO2: Evolution of the average velocity, kinetic energy and parallel momentum



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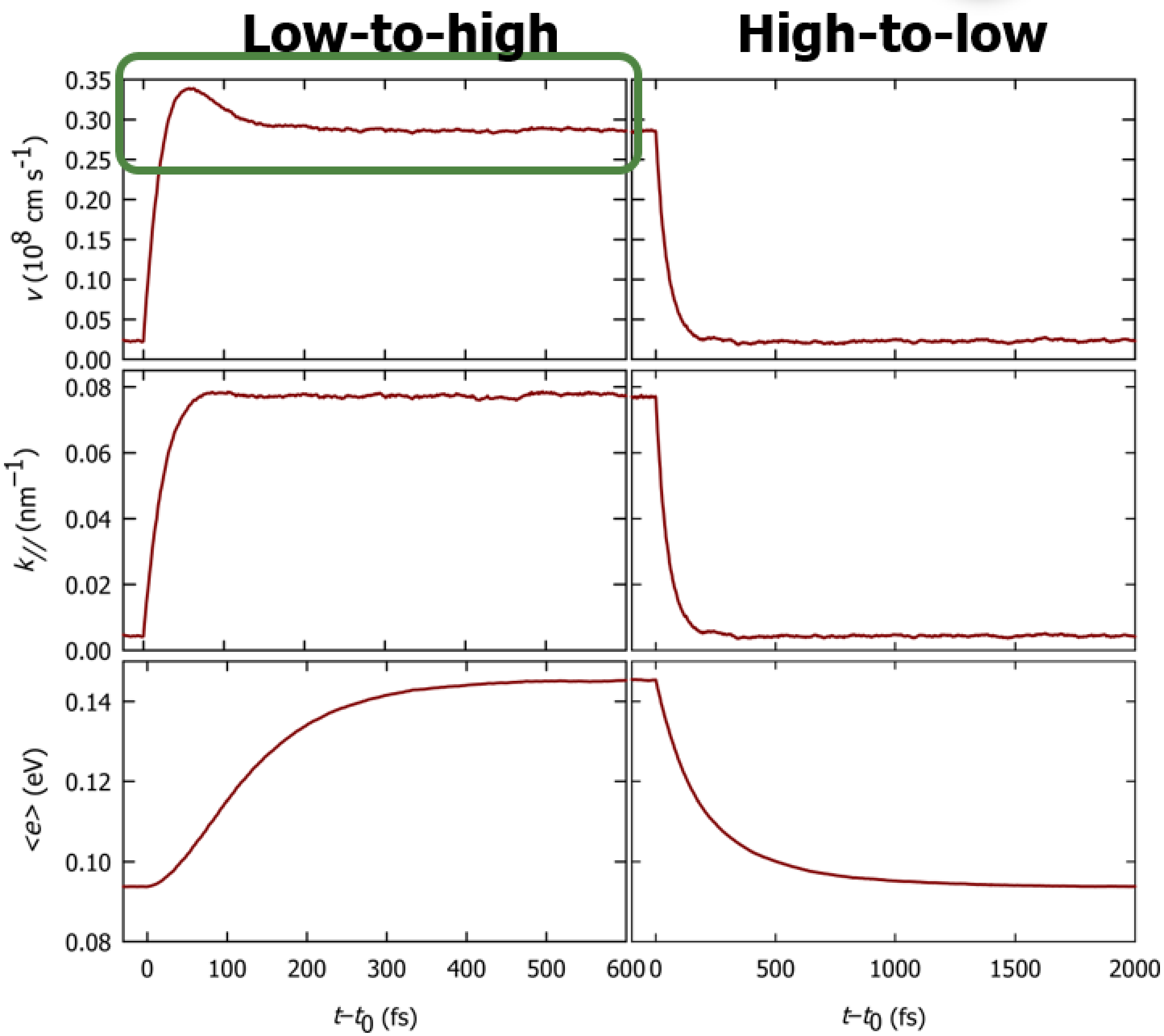

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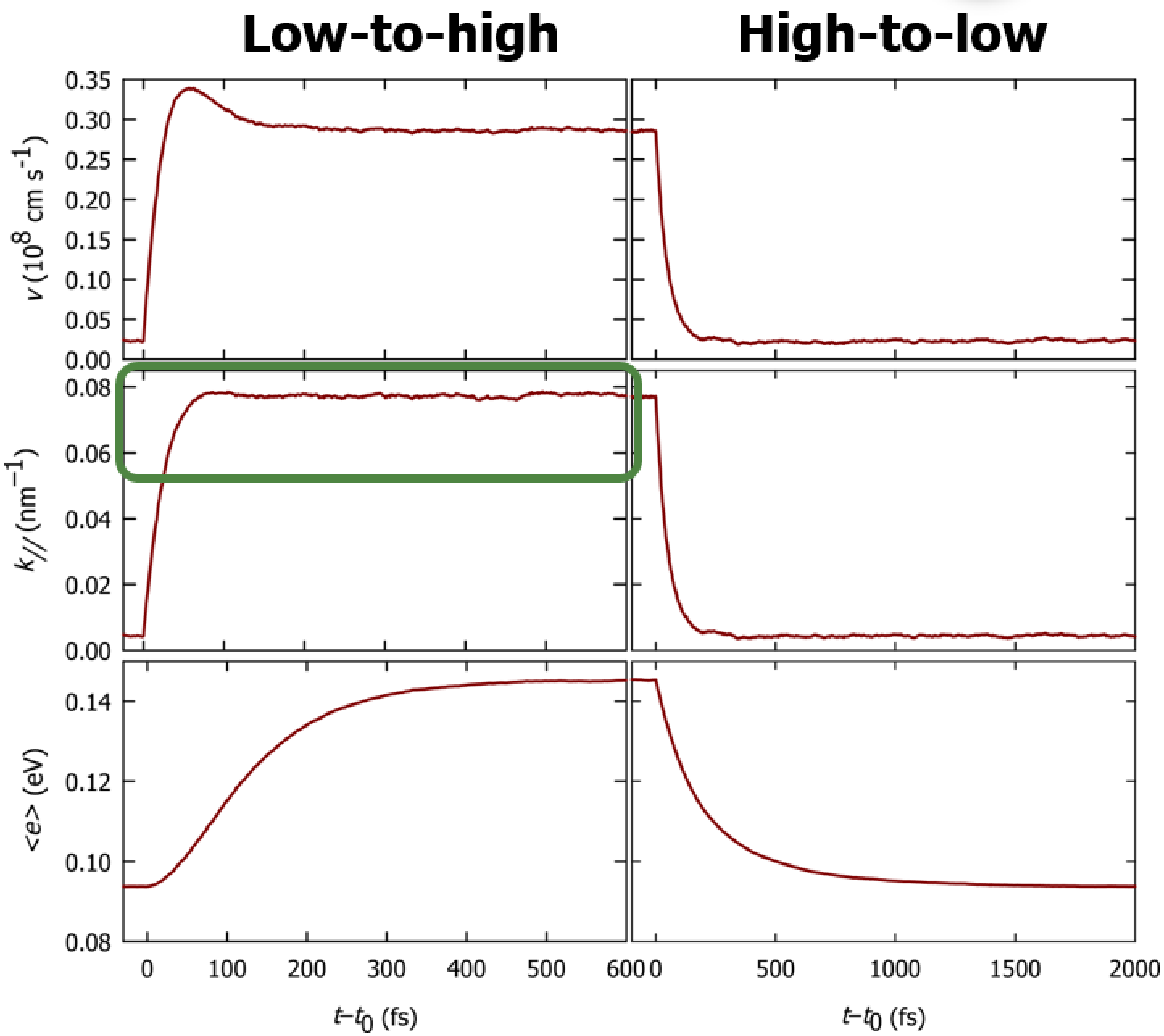

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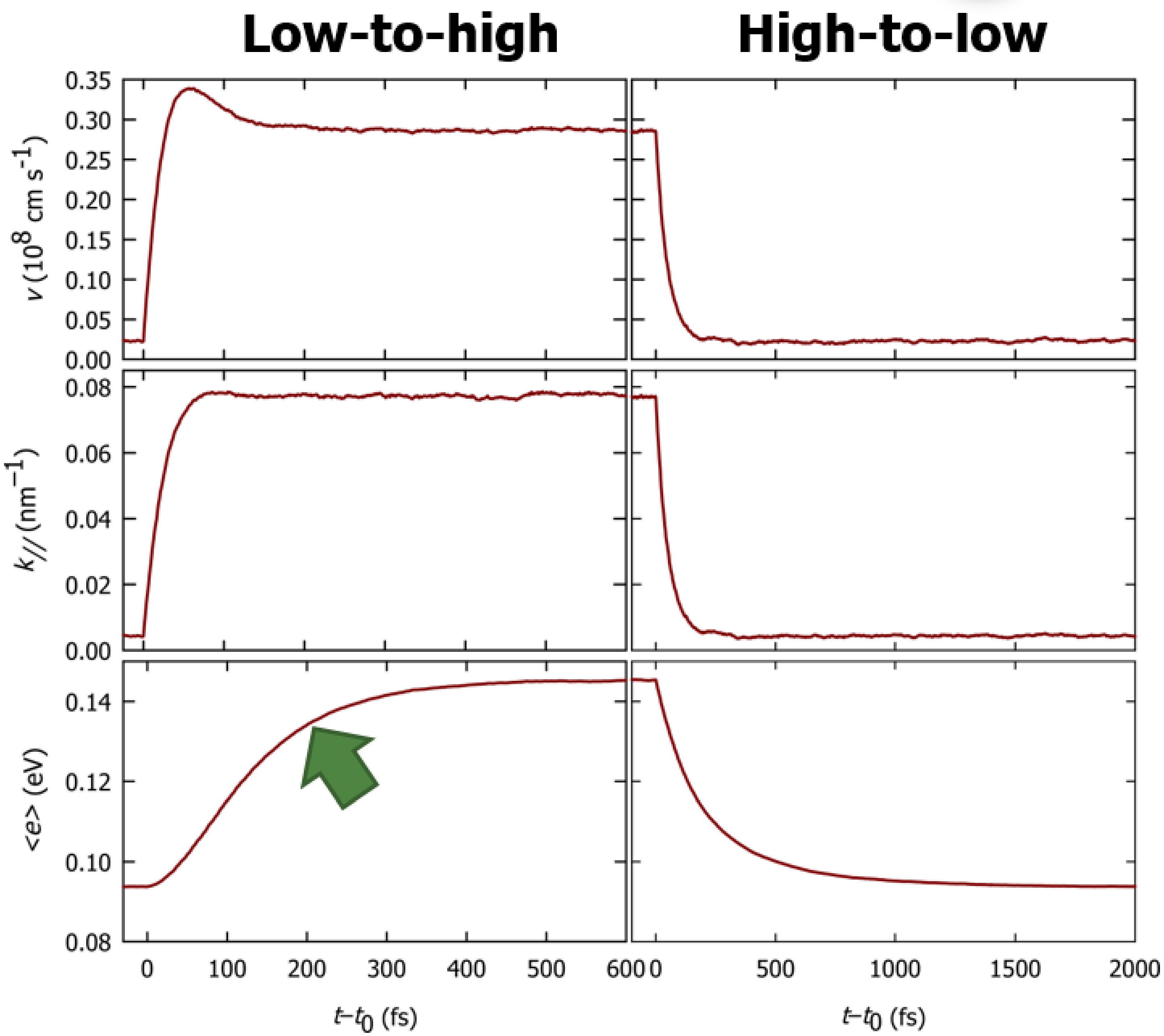

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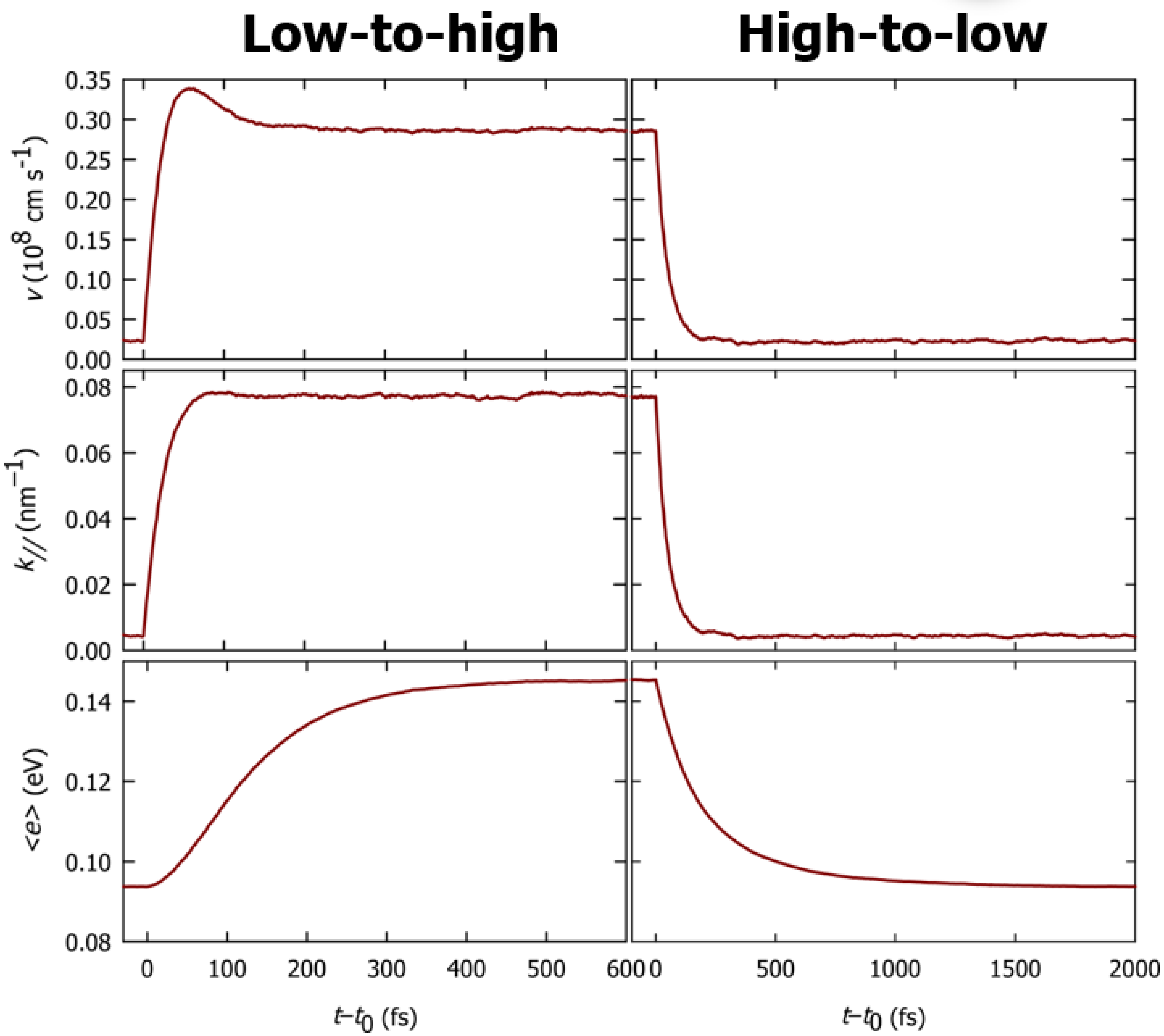

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$$\mathbf{v} = \frac{v_F}{|\mathbf{k}|}\begin{pmatrix} k_x \\ k_y \end{pmatrix}$$

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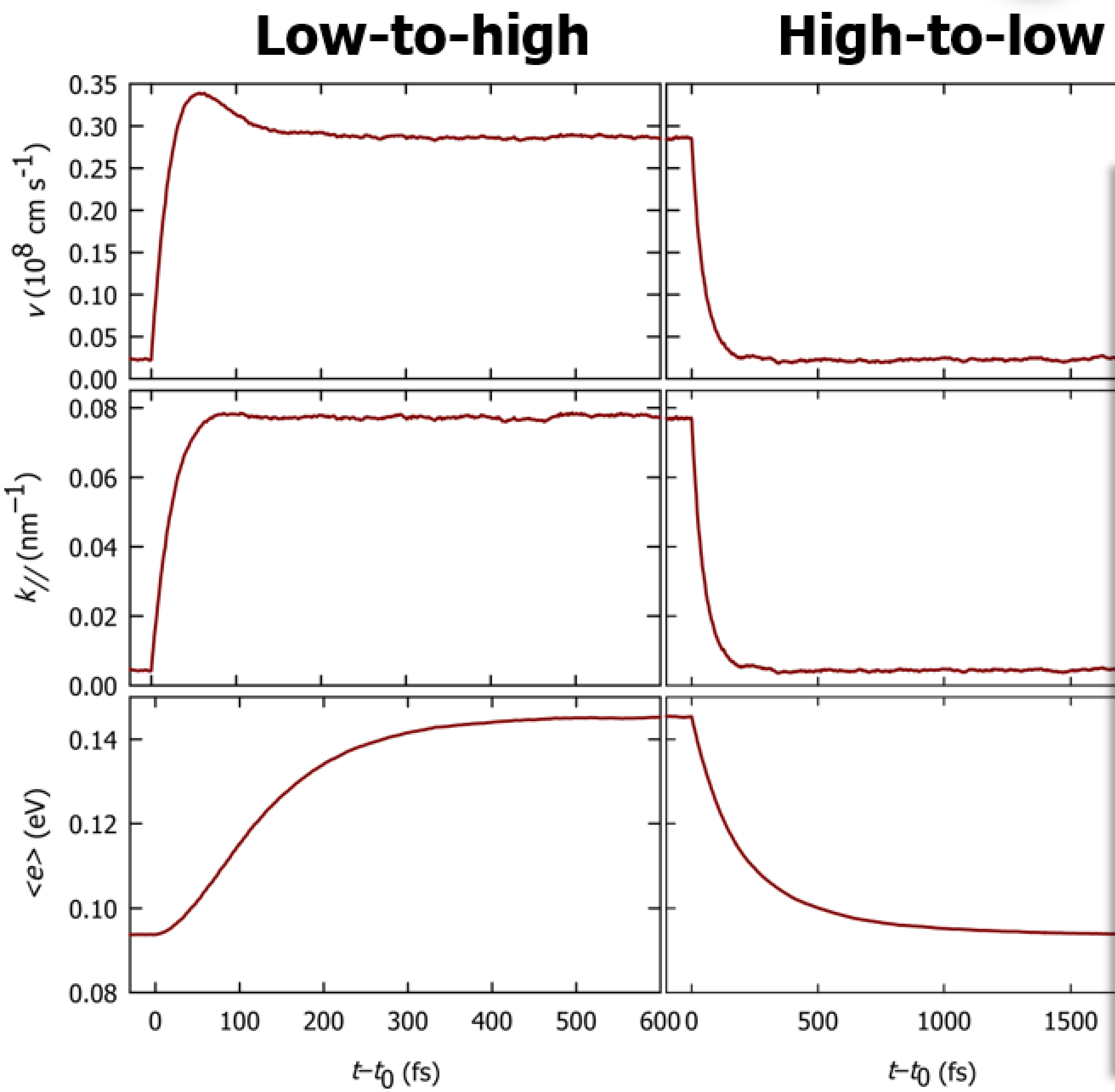

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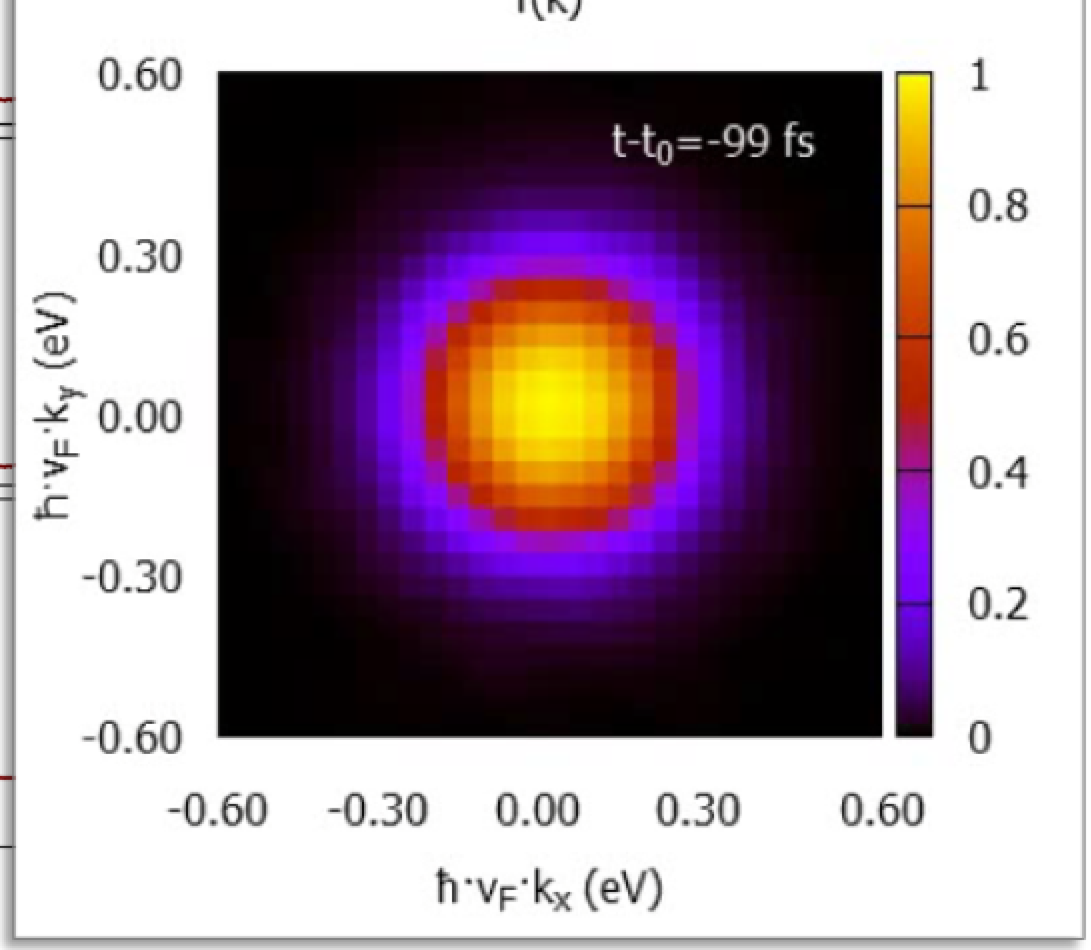

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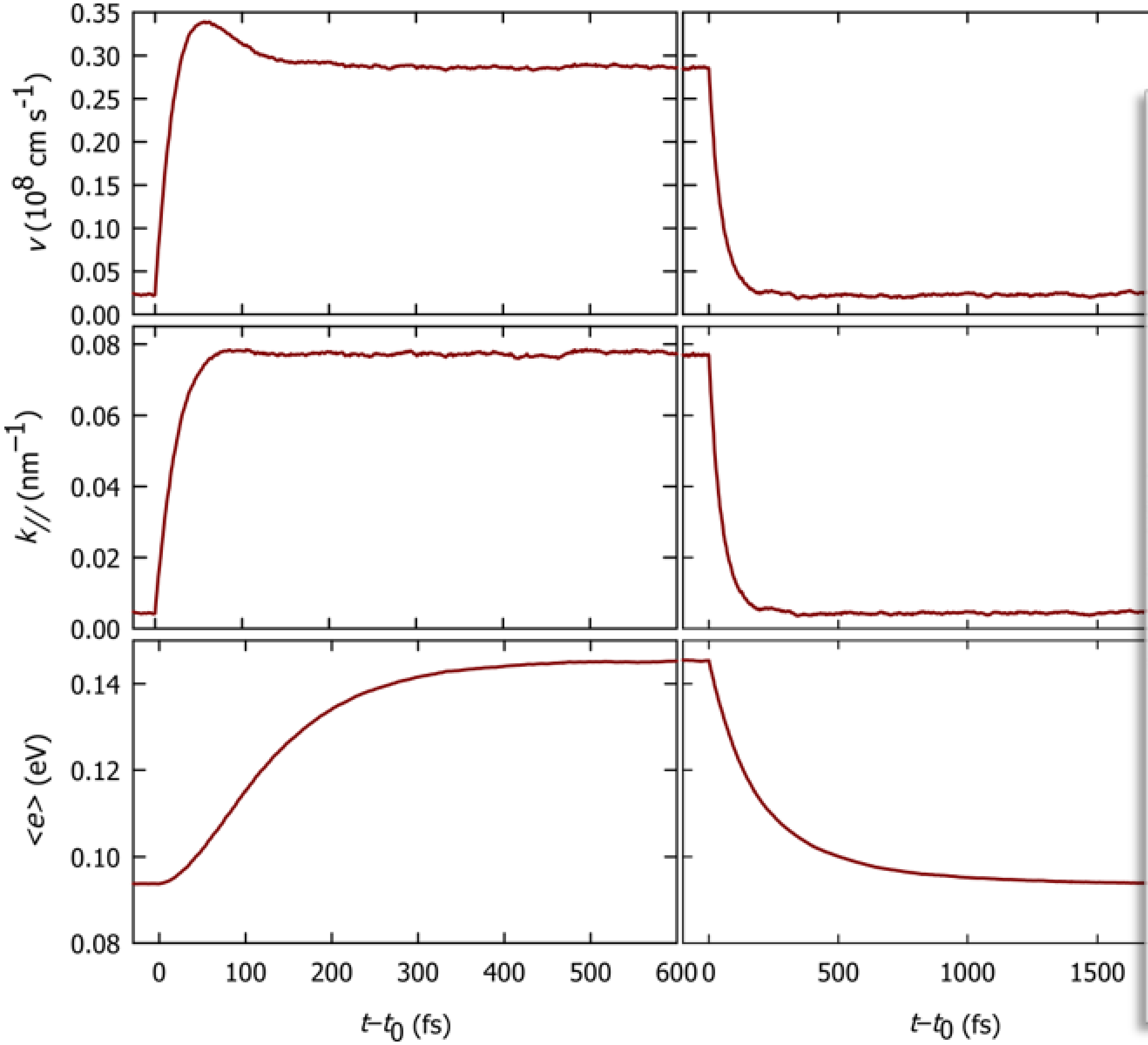
Low-to-high **High-to-low**



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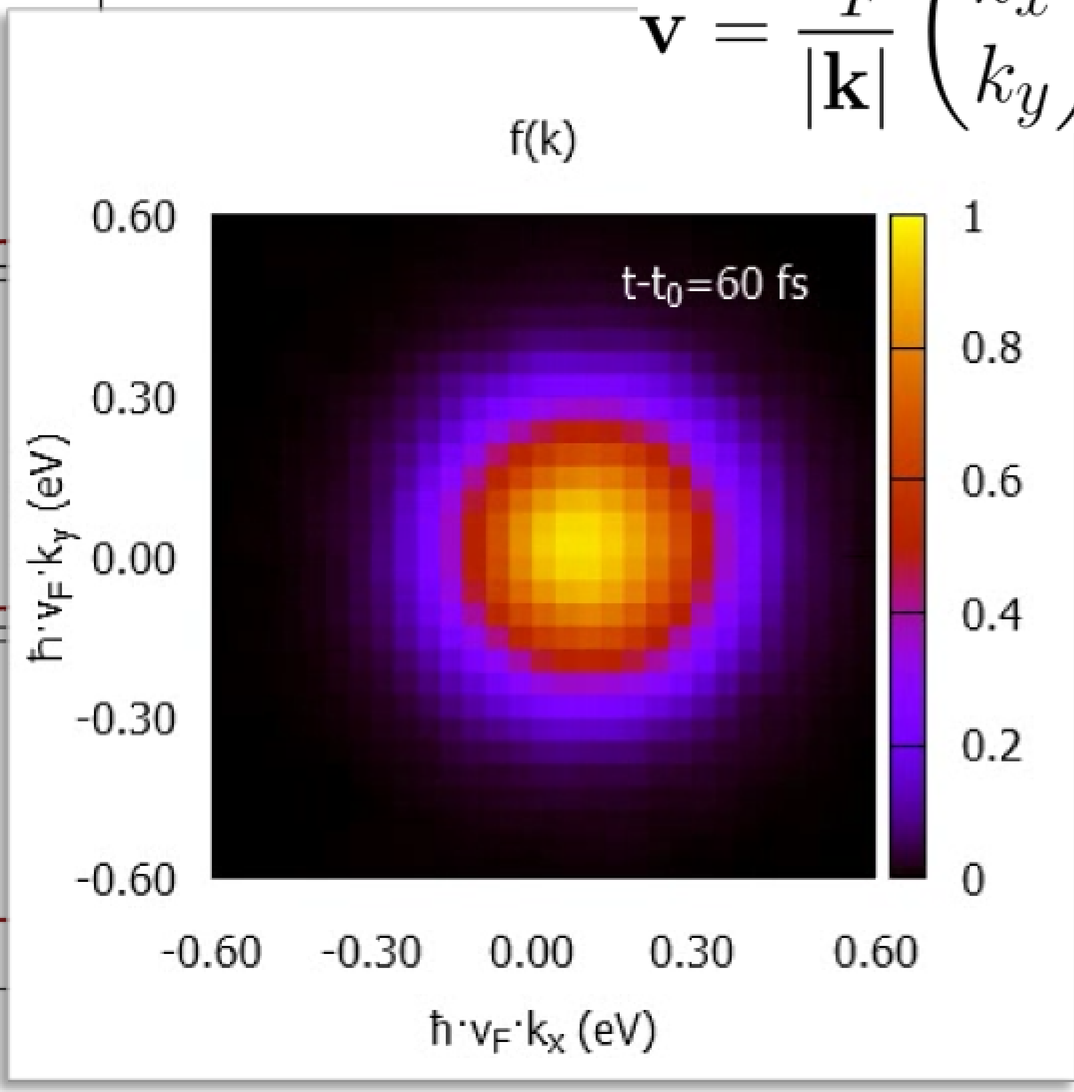

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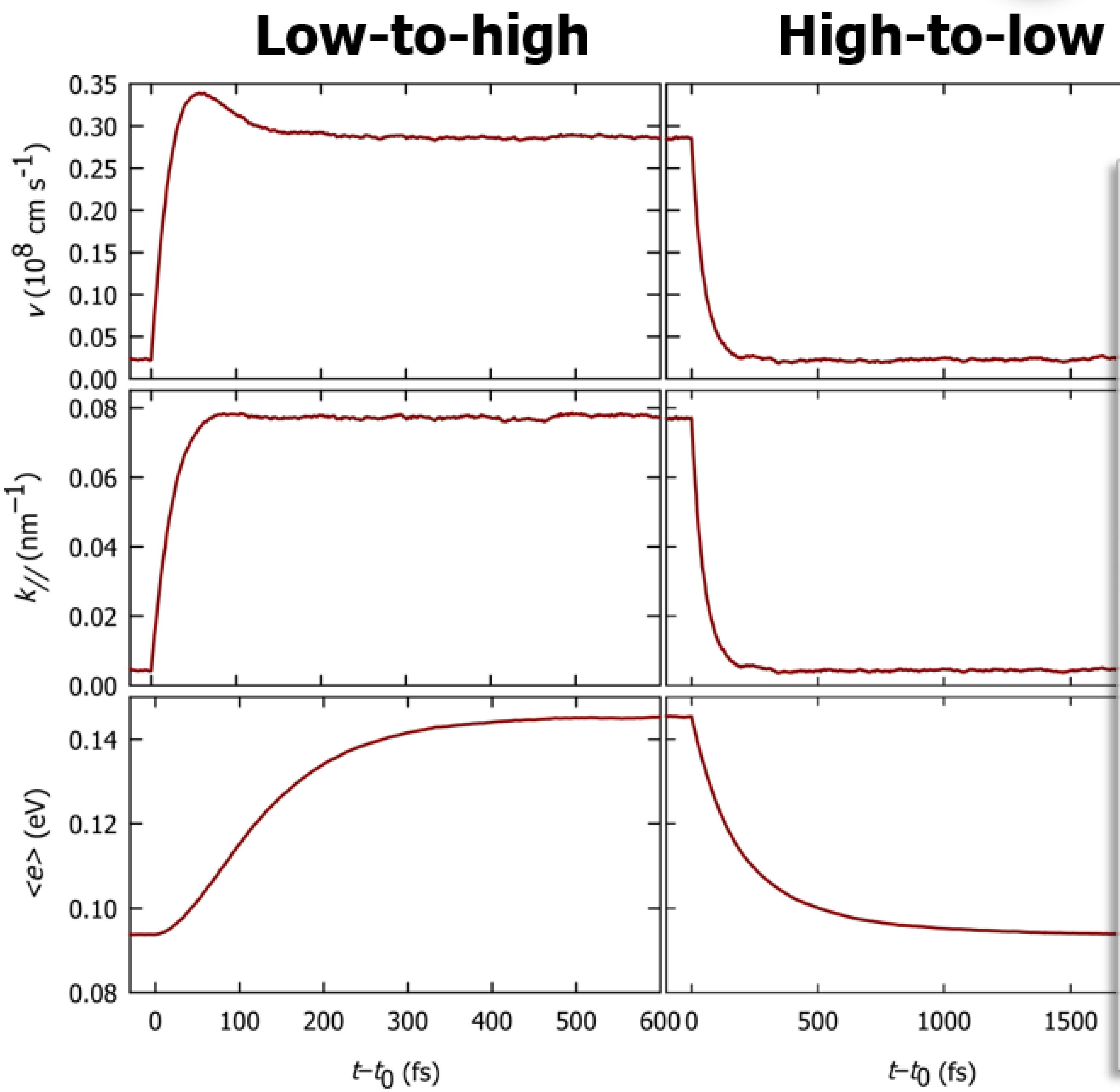

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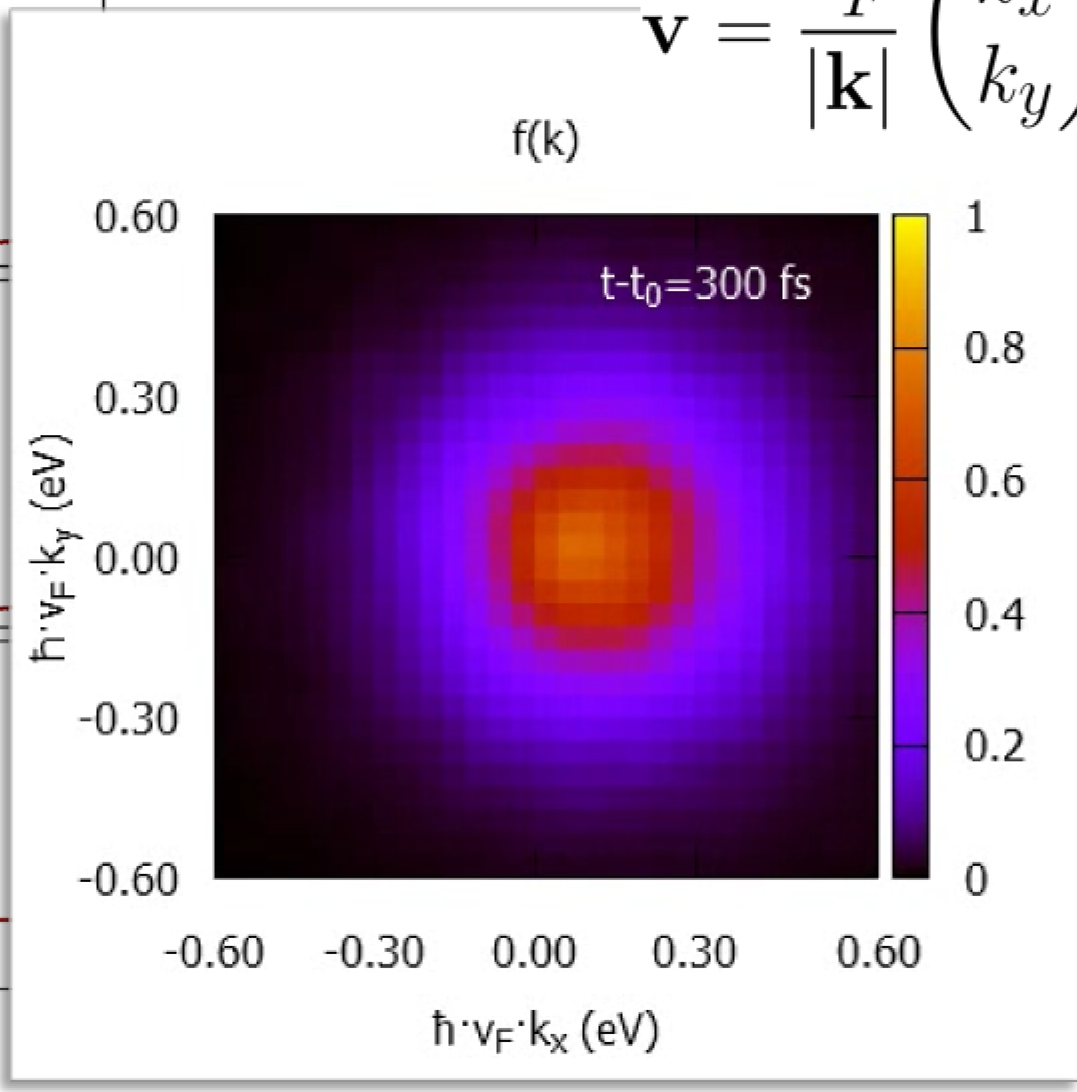

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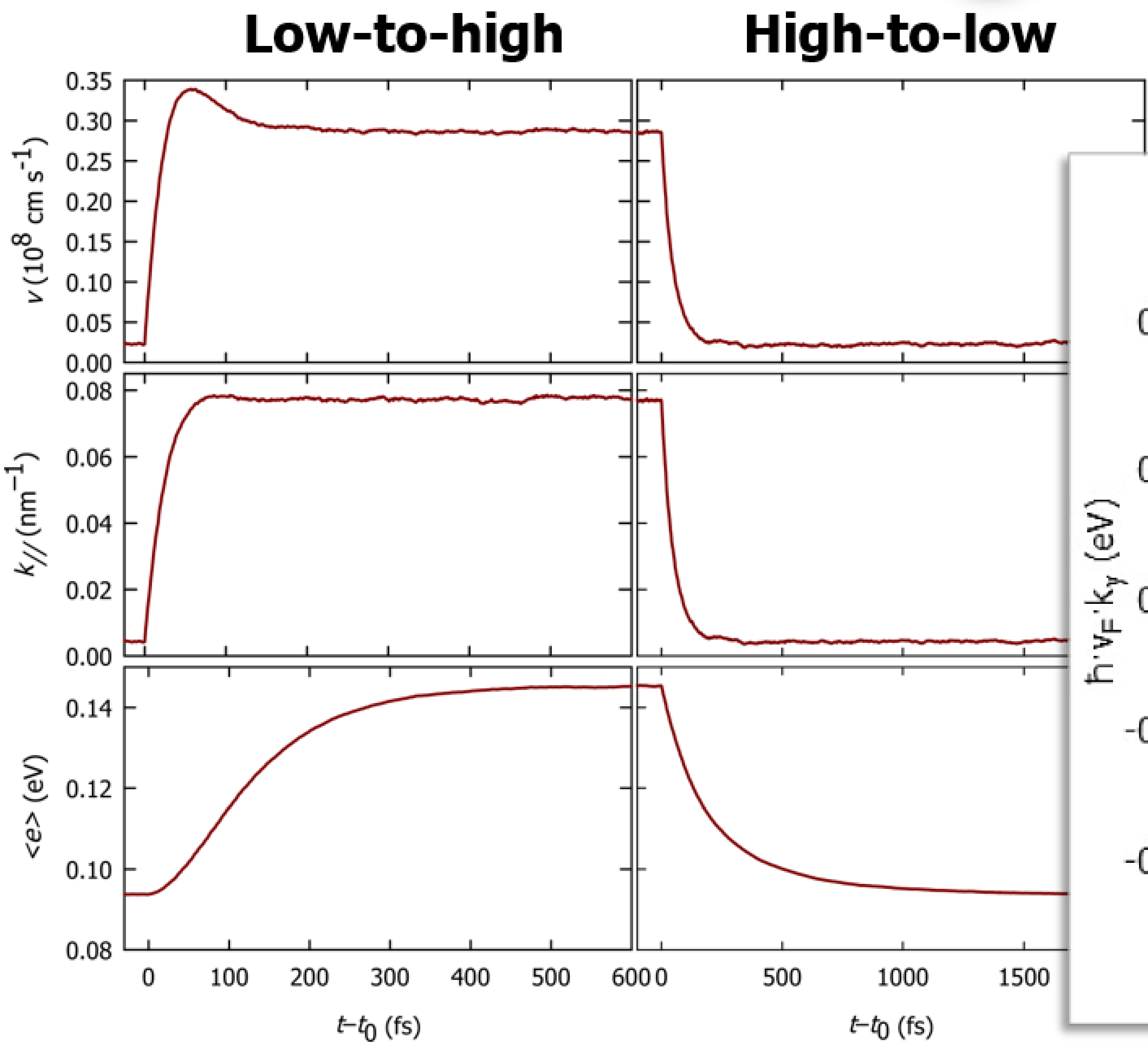

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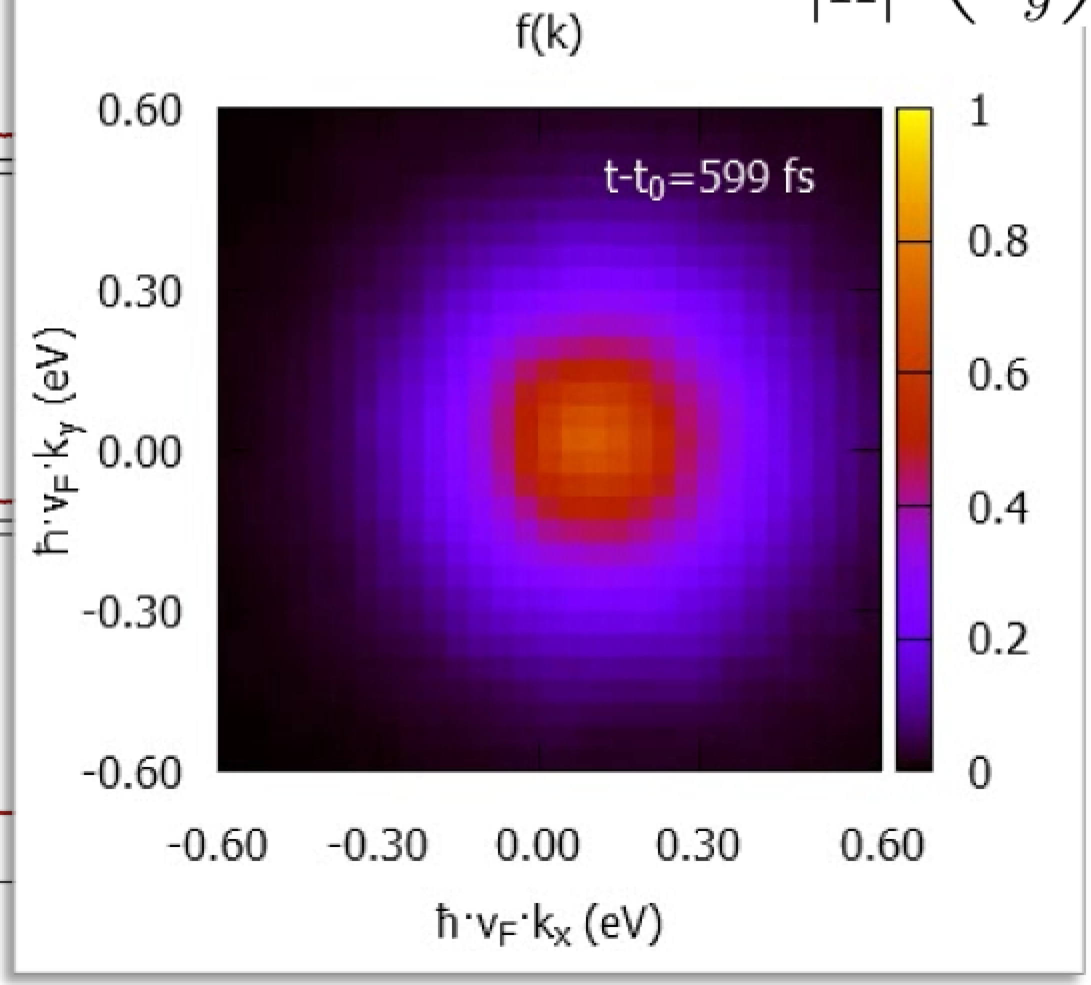
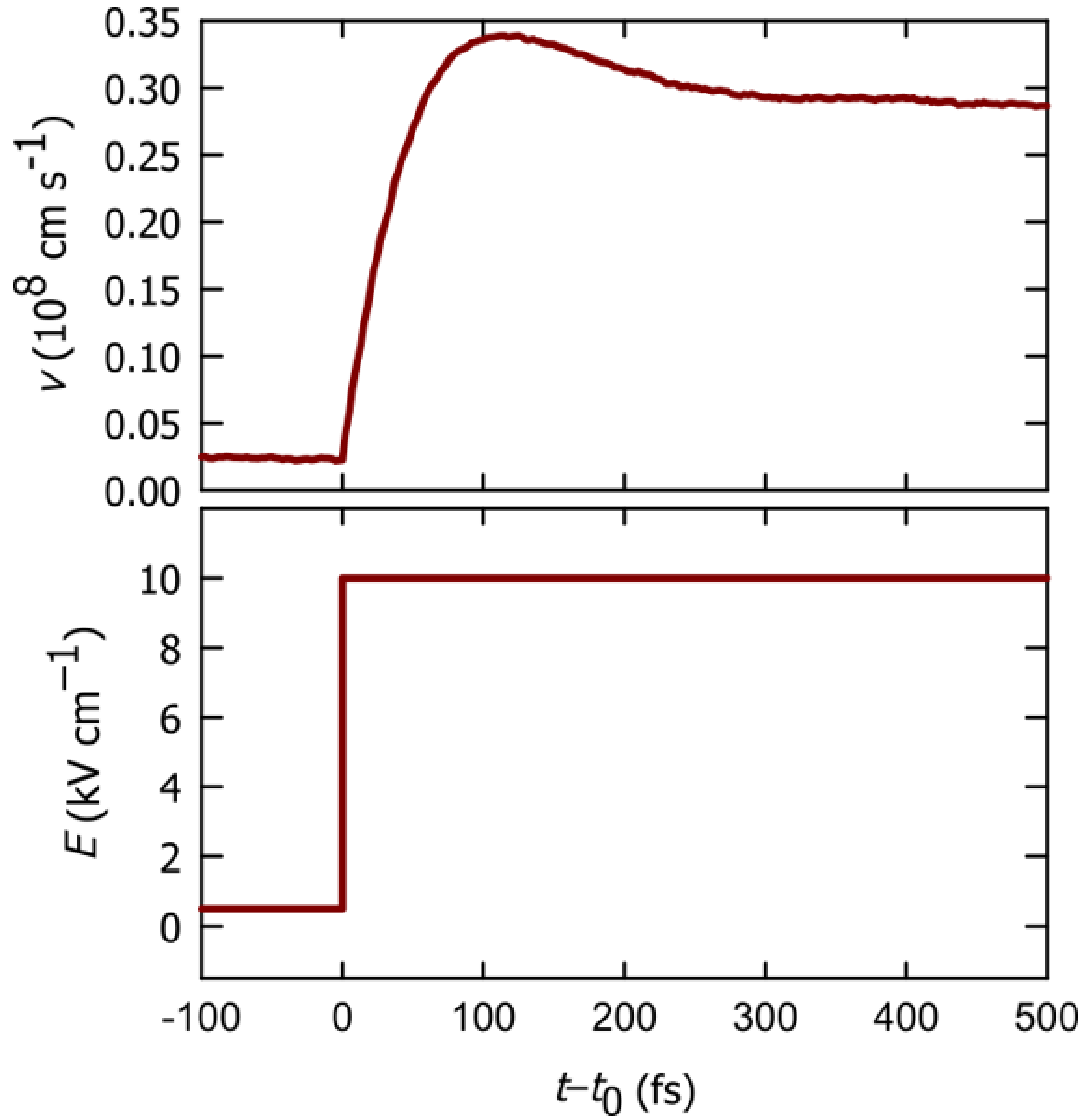


Graphene on SiO2; **low to high** field: Transient Autocorrelation Function



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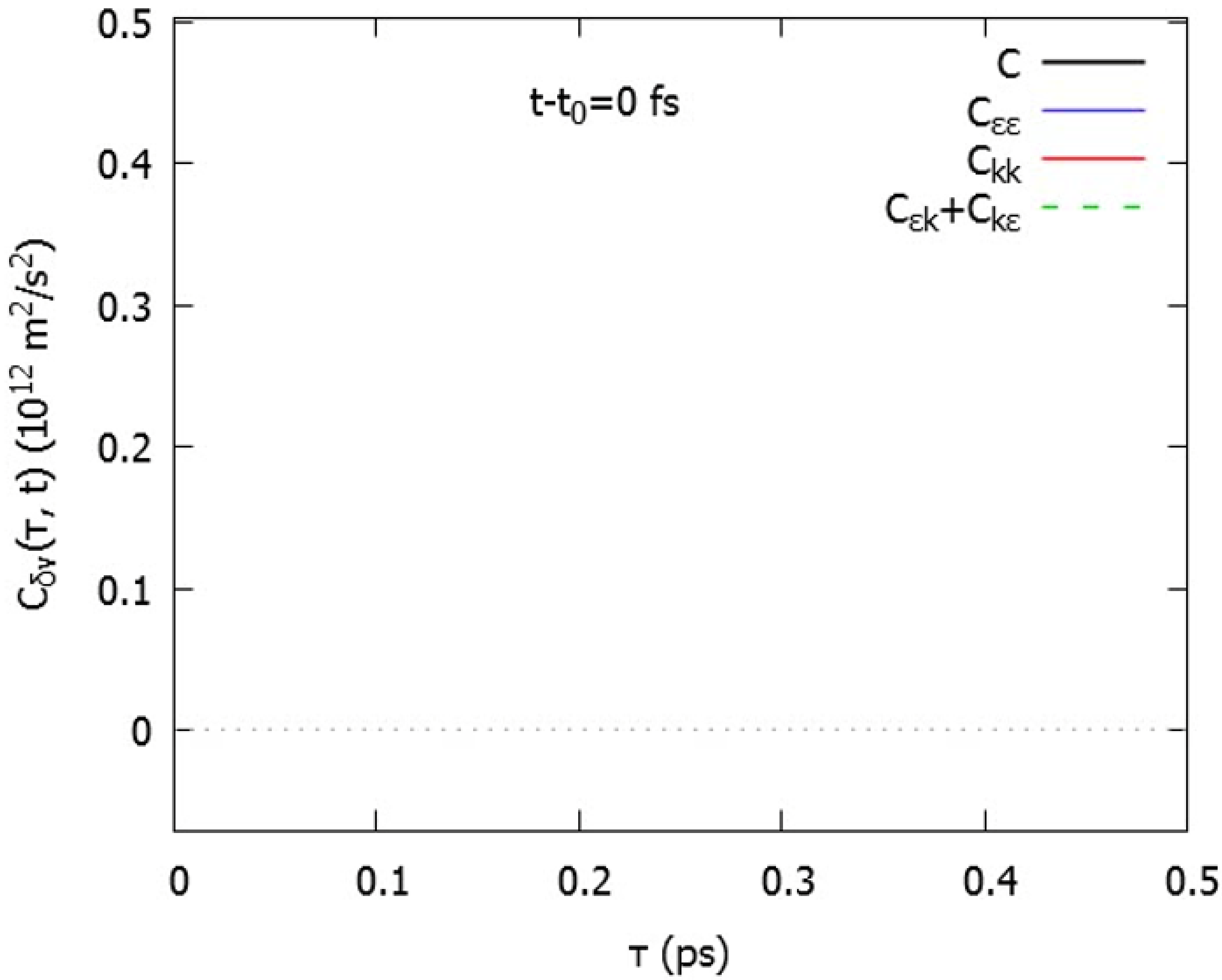
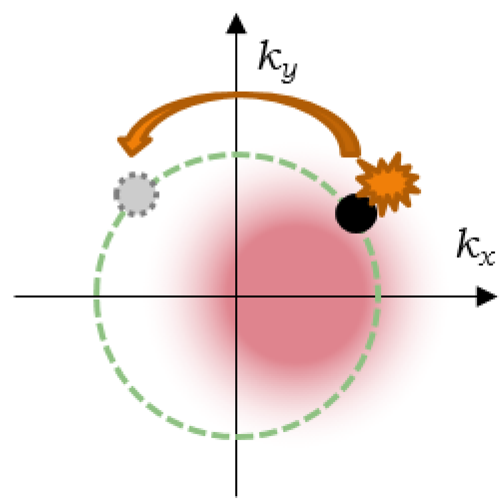


C_{kk}

Fast change in the fluctuation sign as a consequence of fast momentum (velocity) reorientation:

- Dragging of the electric field
- ↑↑ Energy → ↑↑ Scattering



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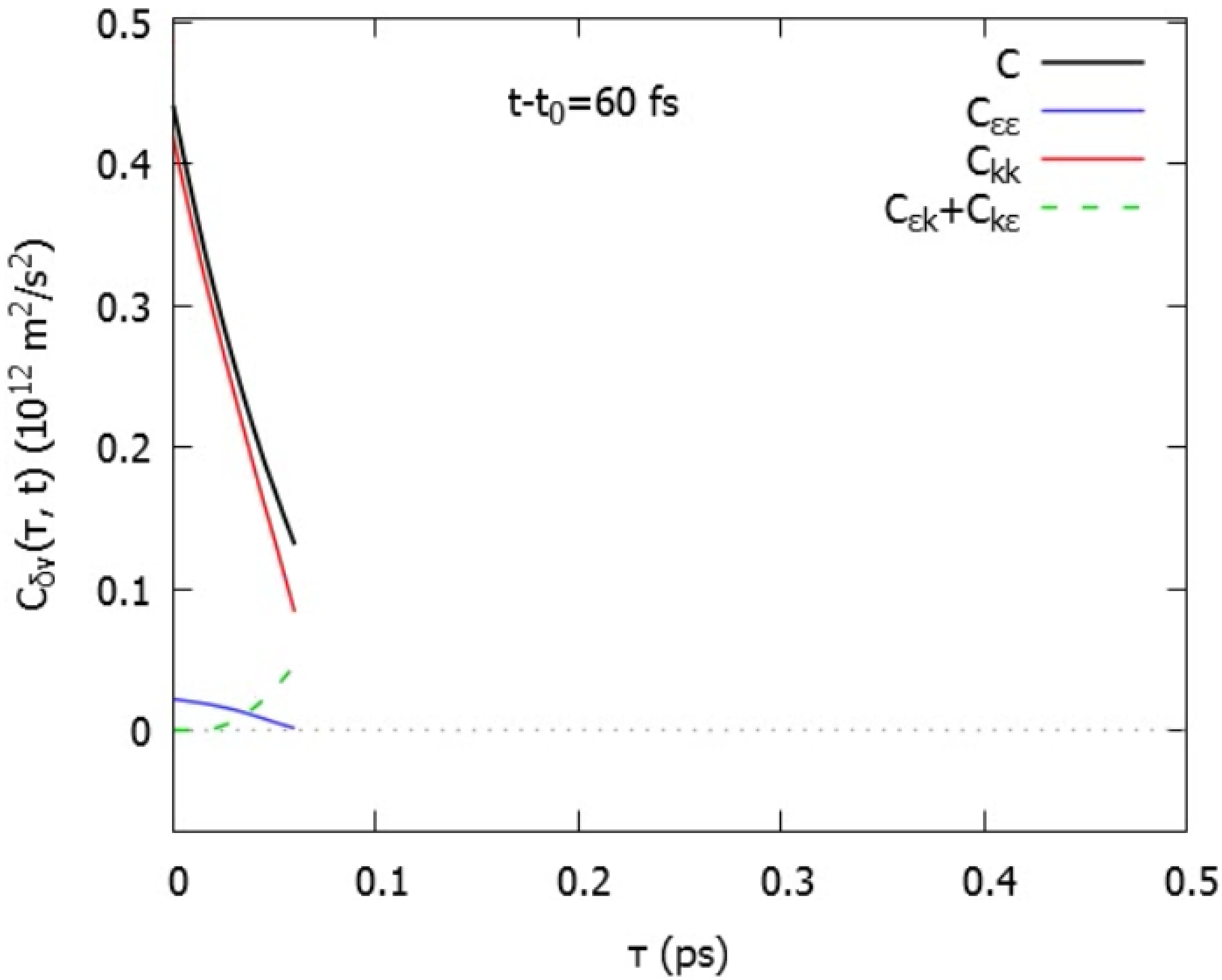

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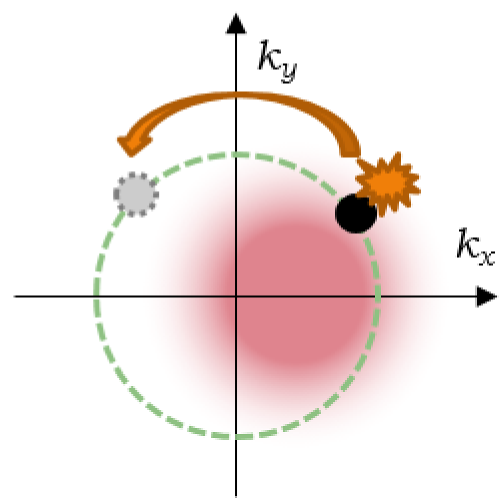

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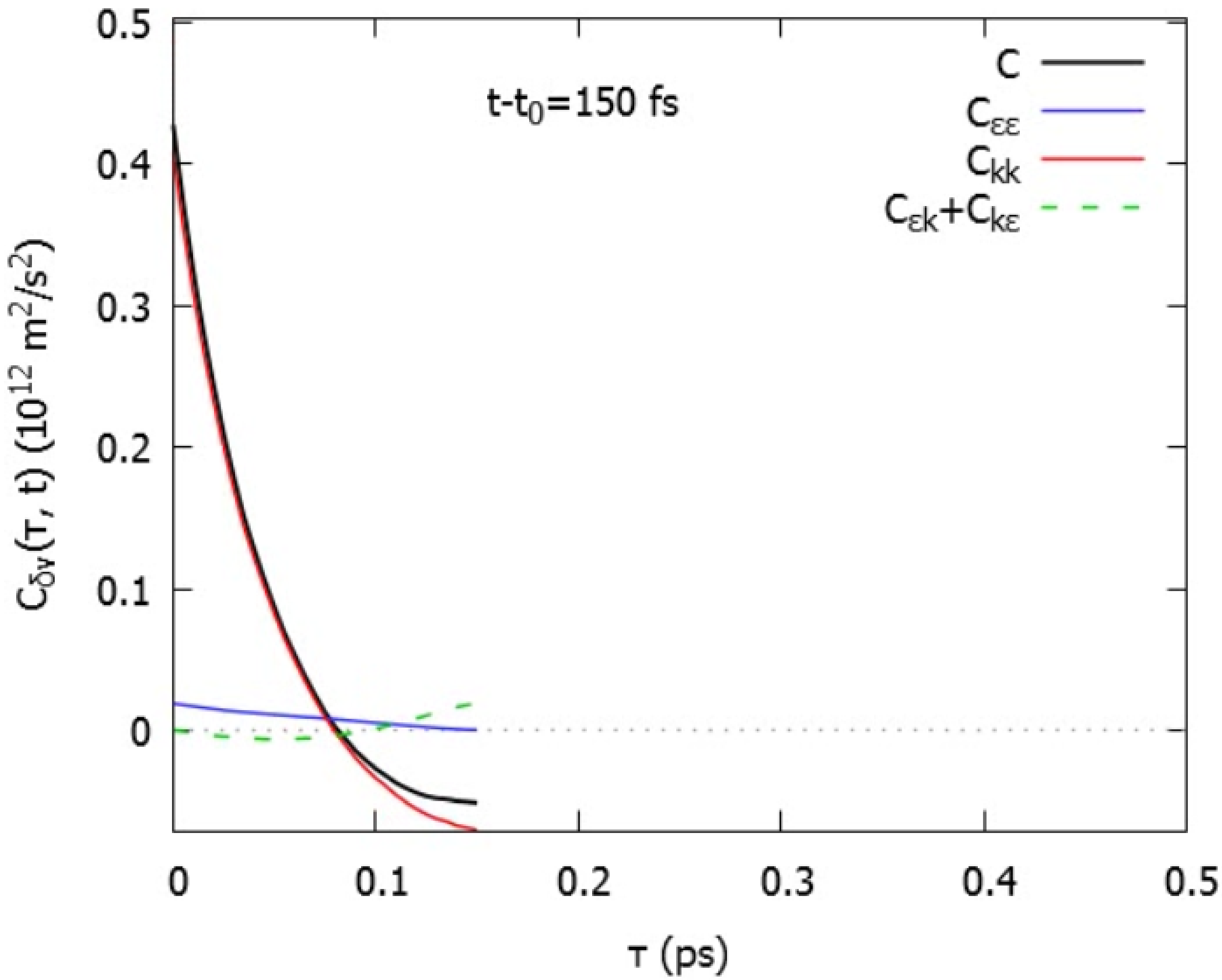

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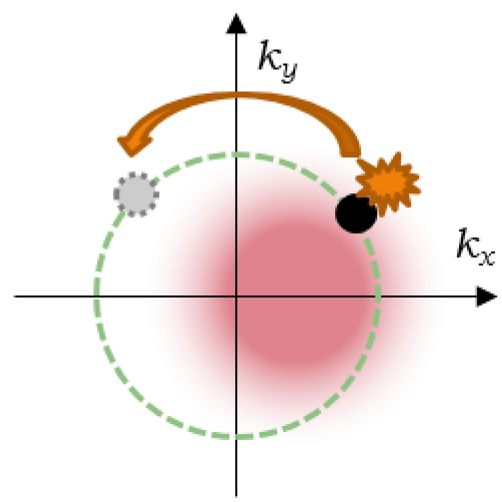

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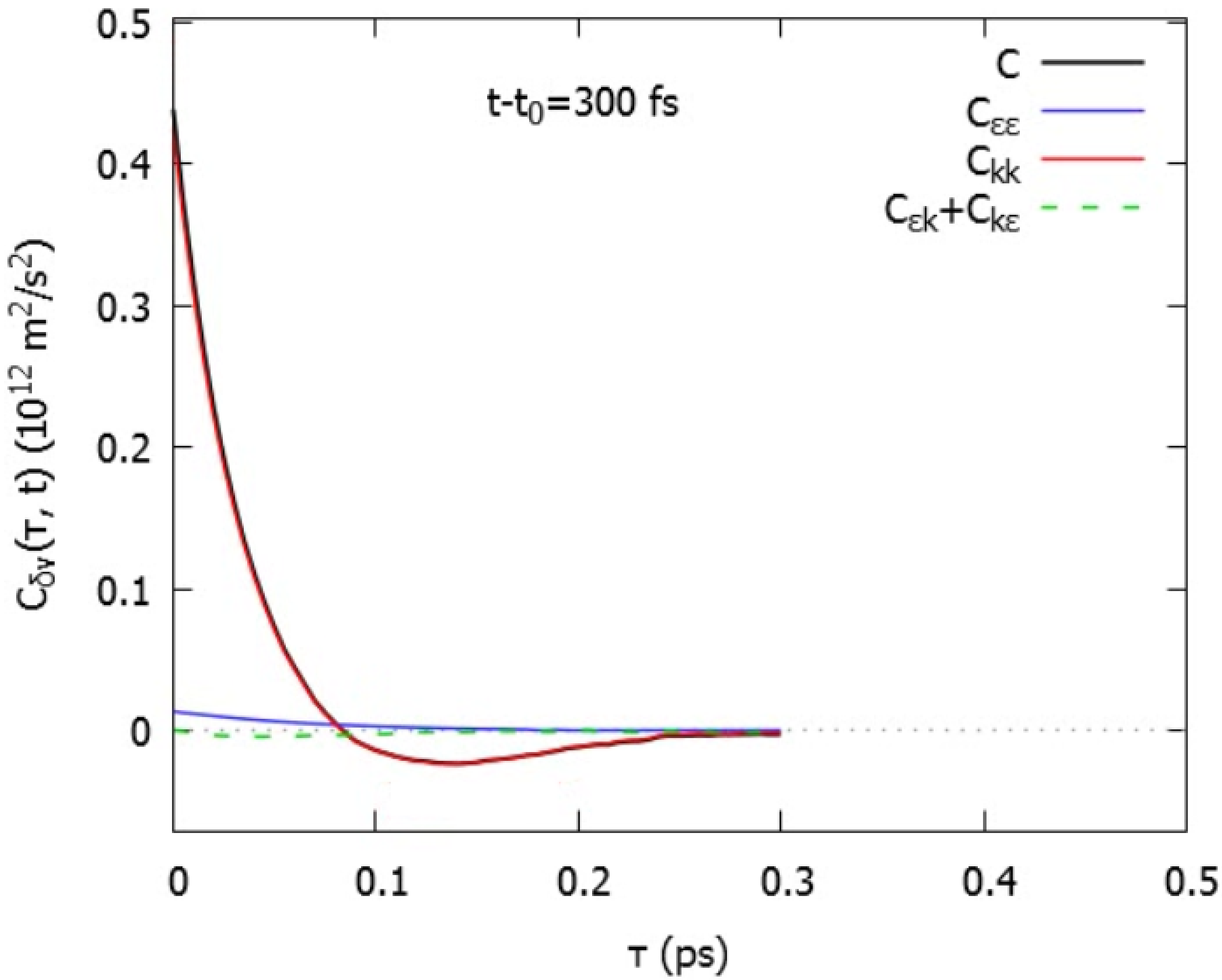

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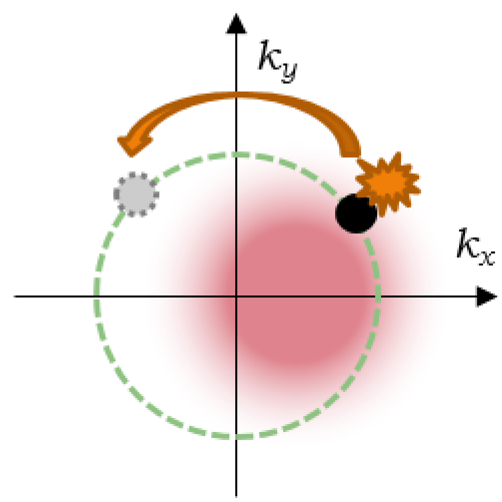

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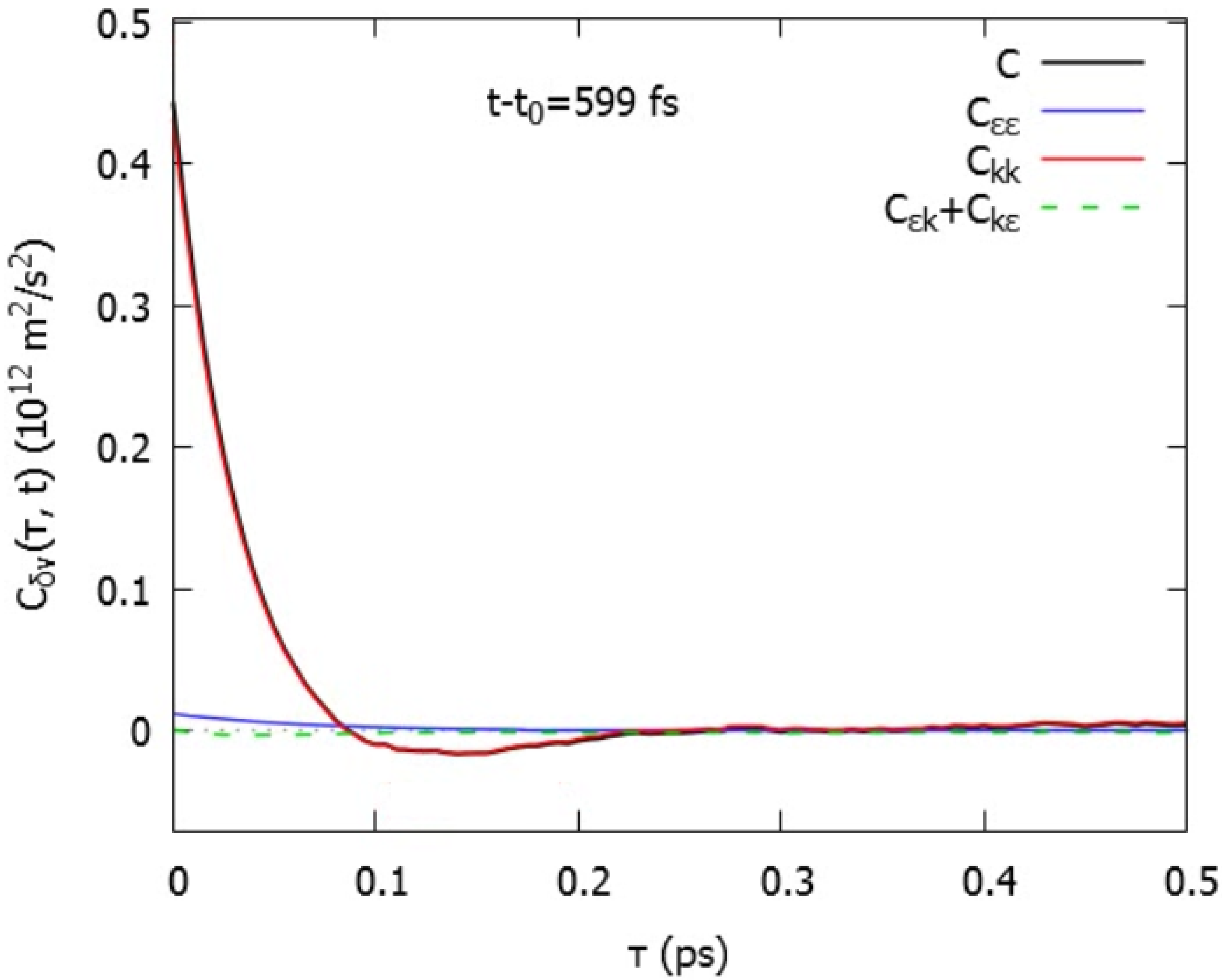

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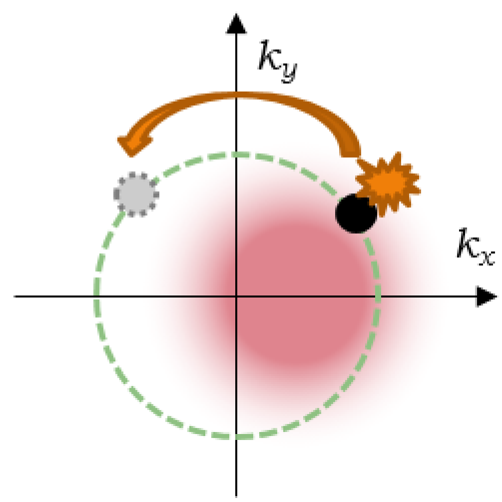

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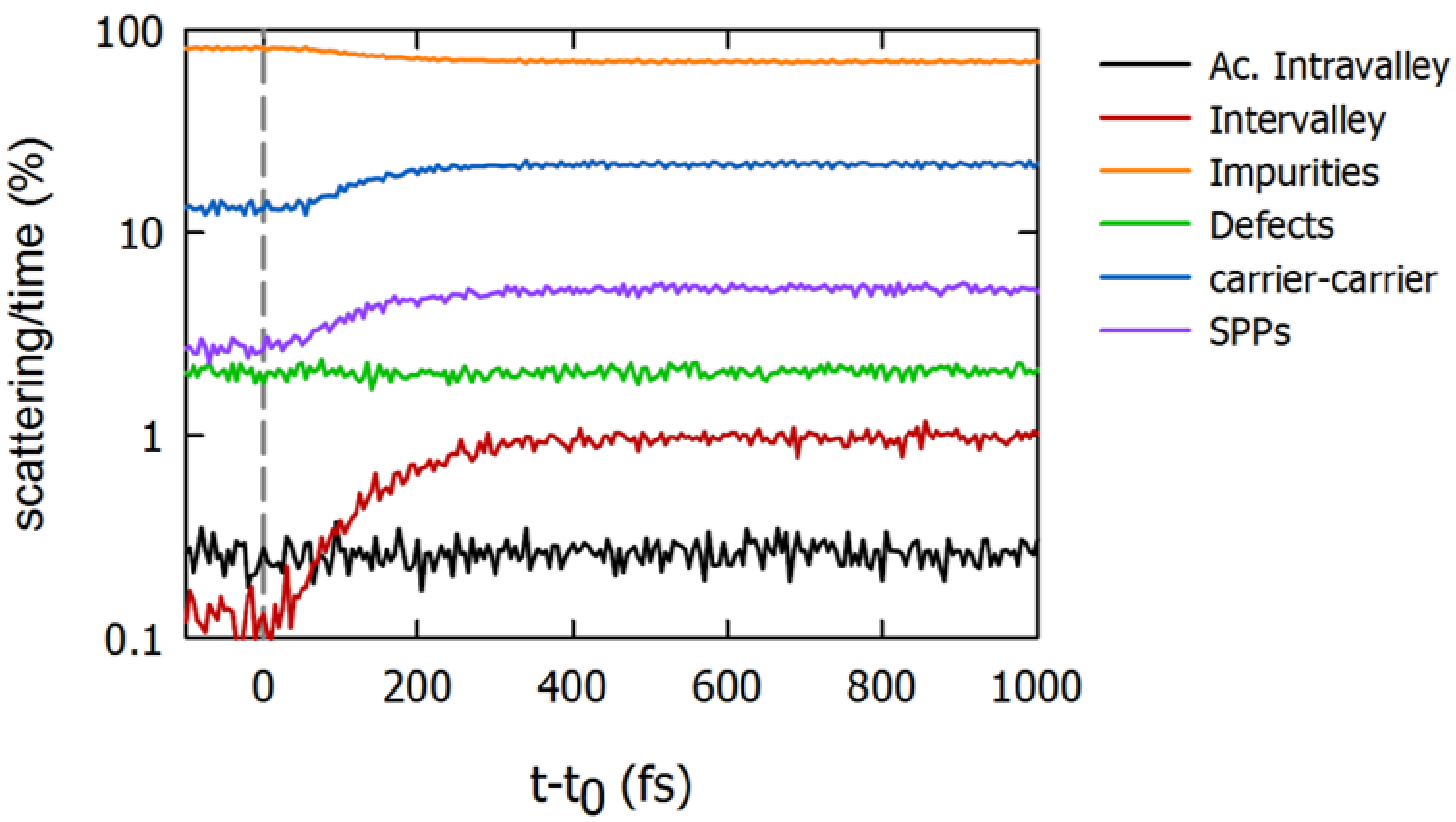

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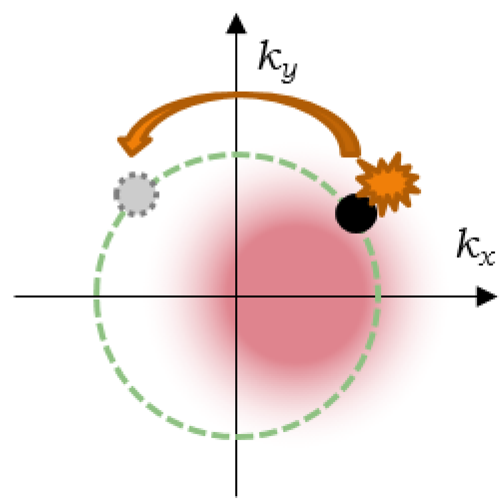

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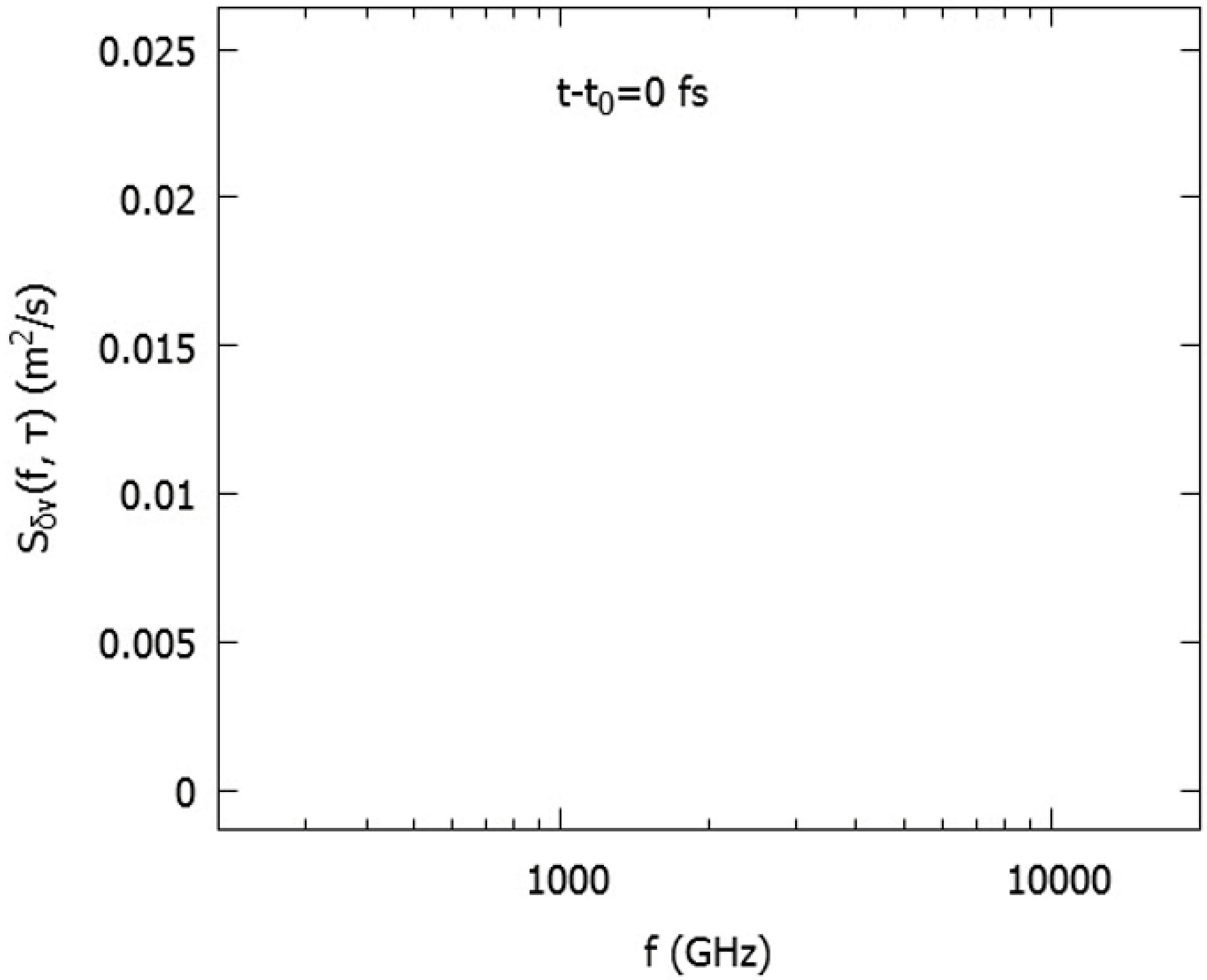

- Lorentzian shape up to 160 fs (Correlation minimum)
- Maximum starts to appear from them on at *f*=2200 GHz

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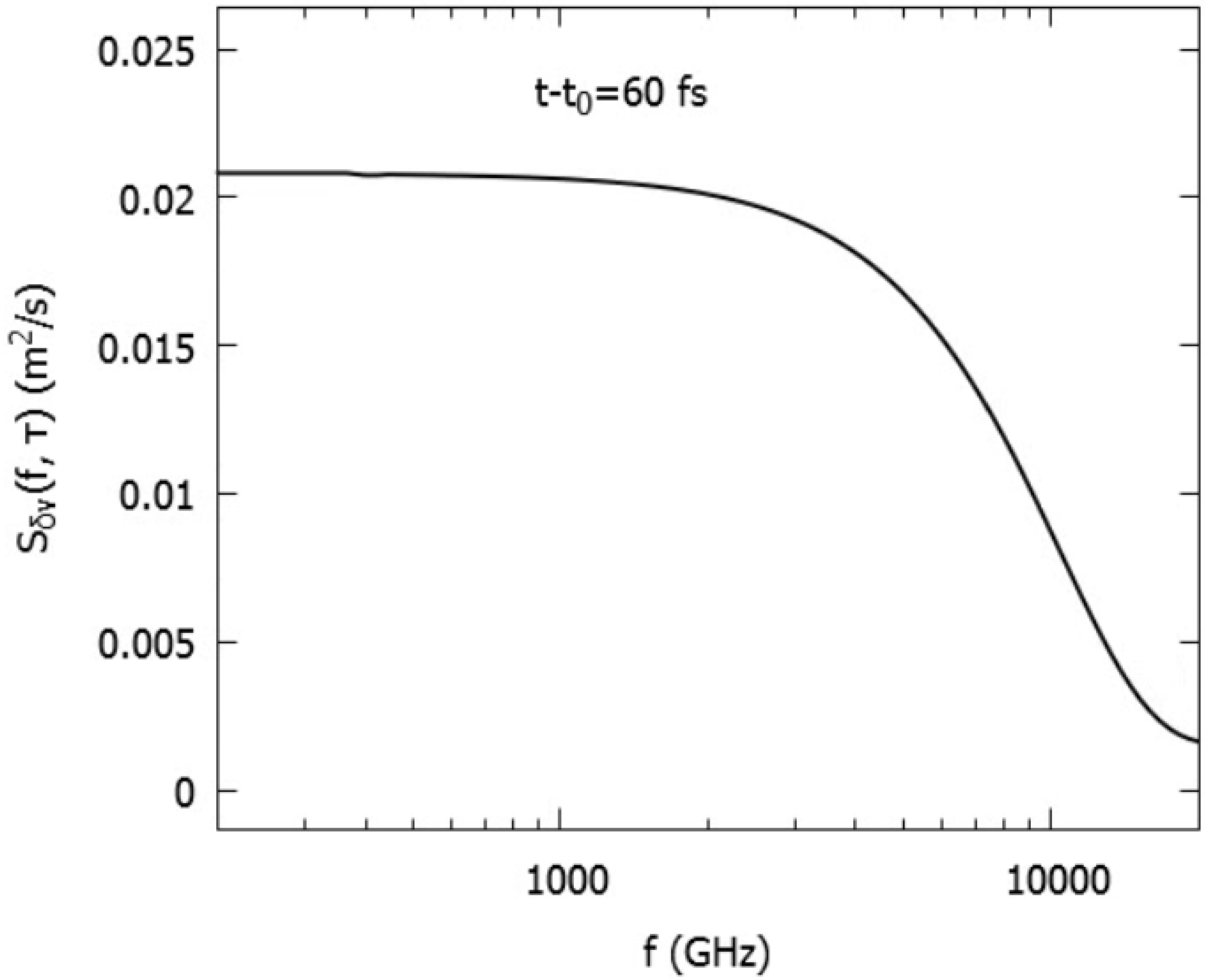

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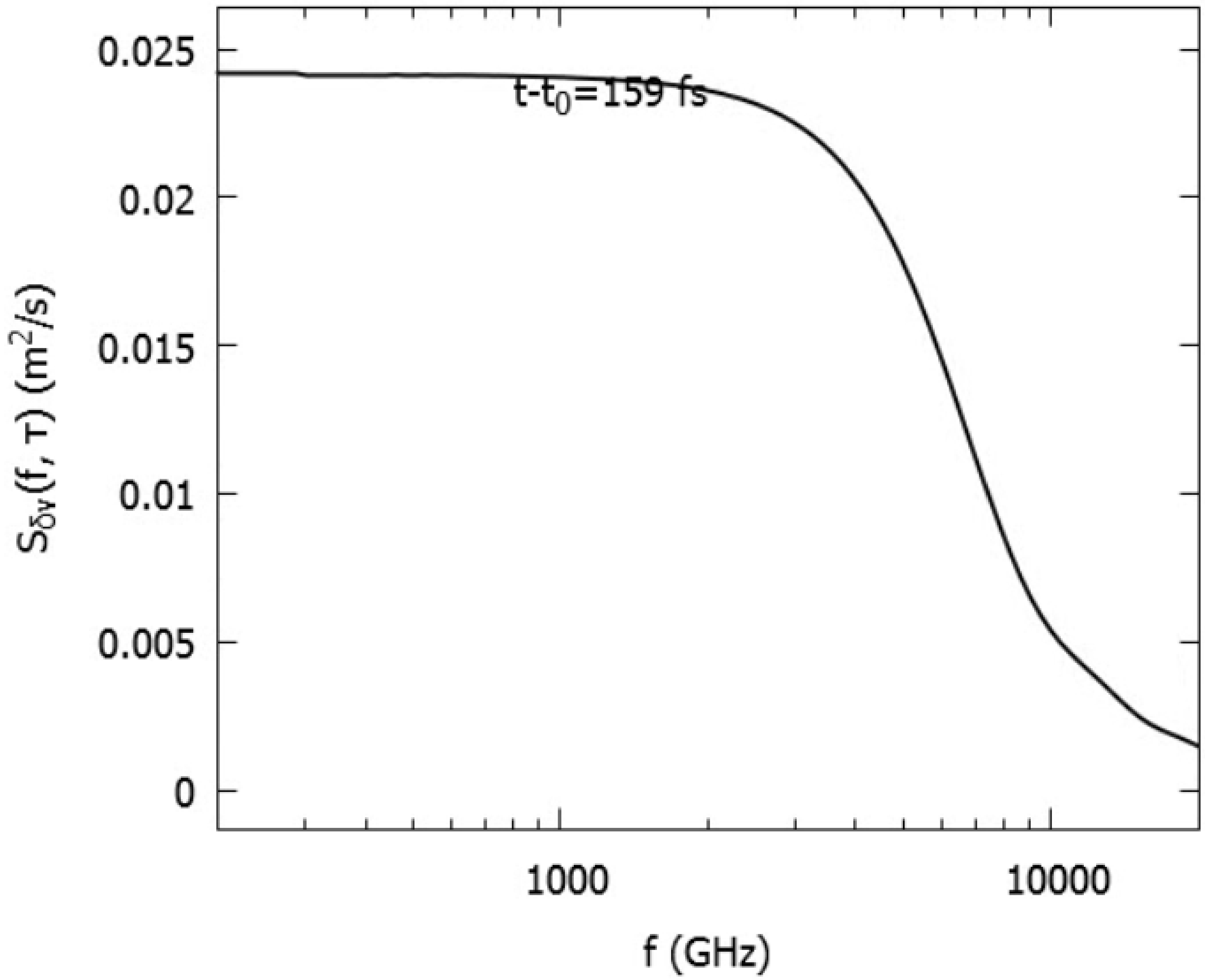

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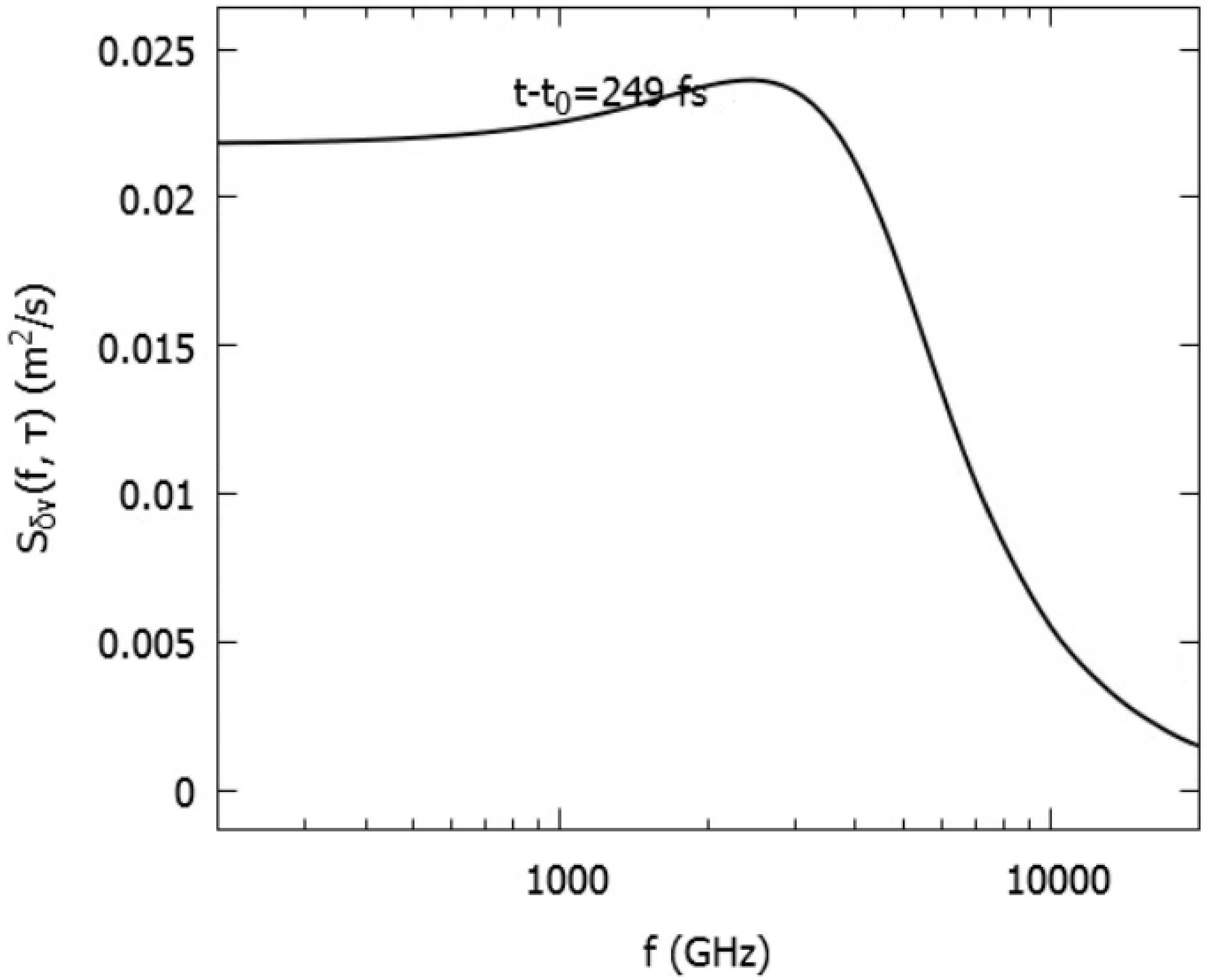

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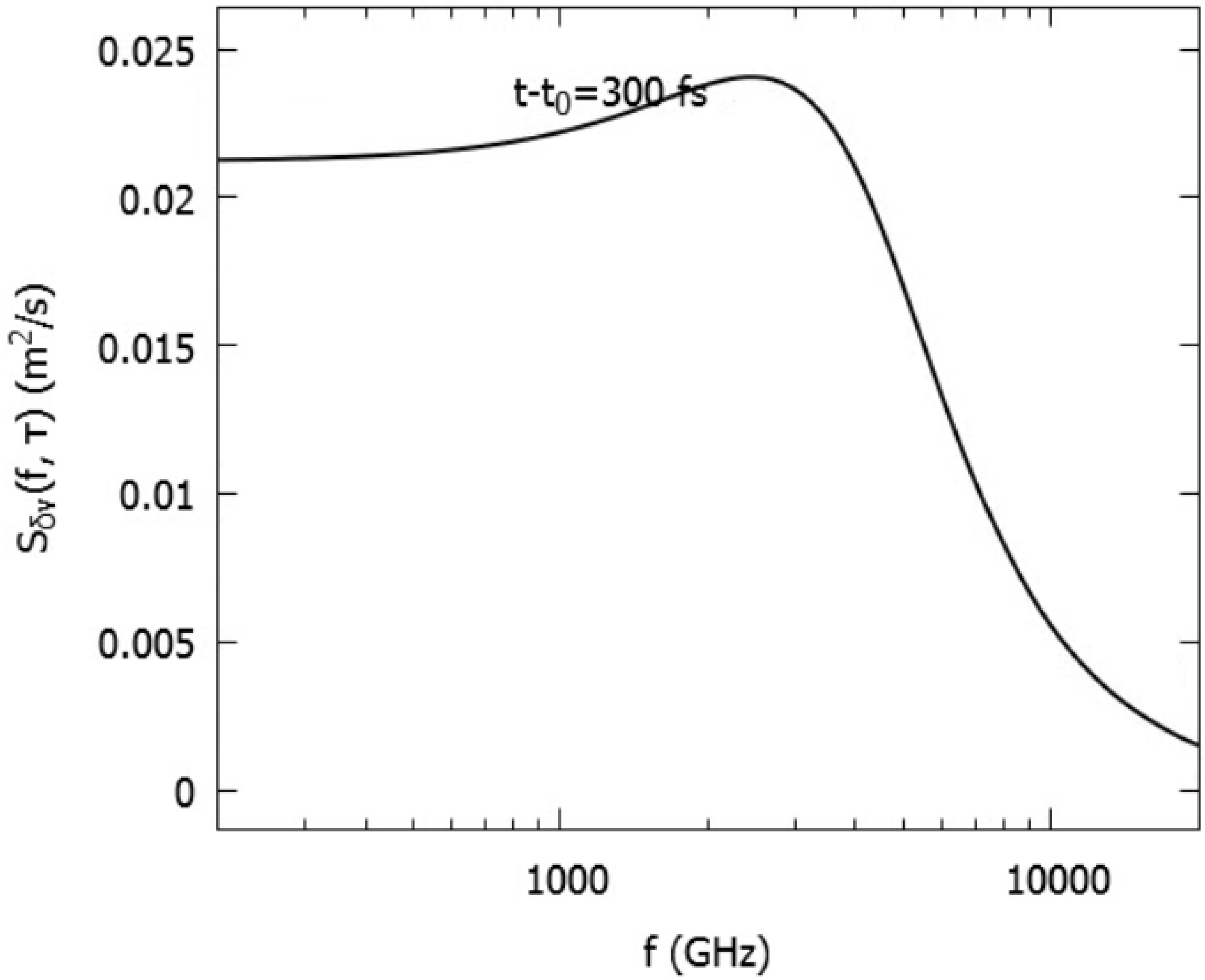

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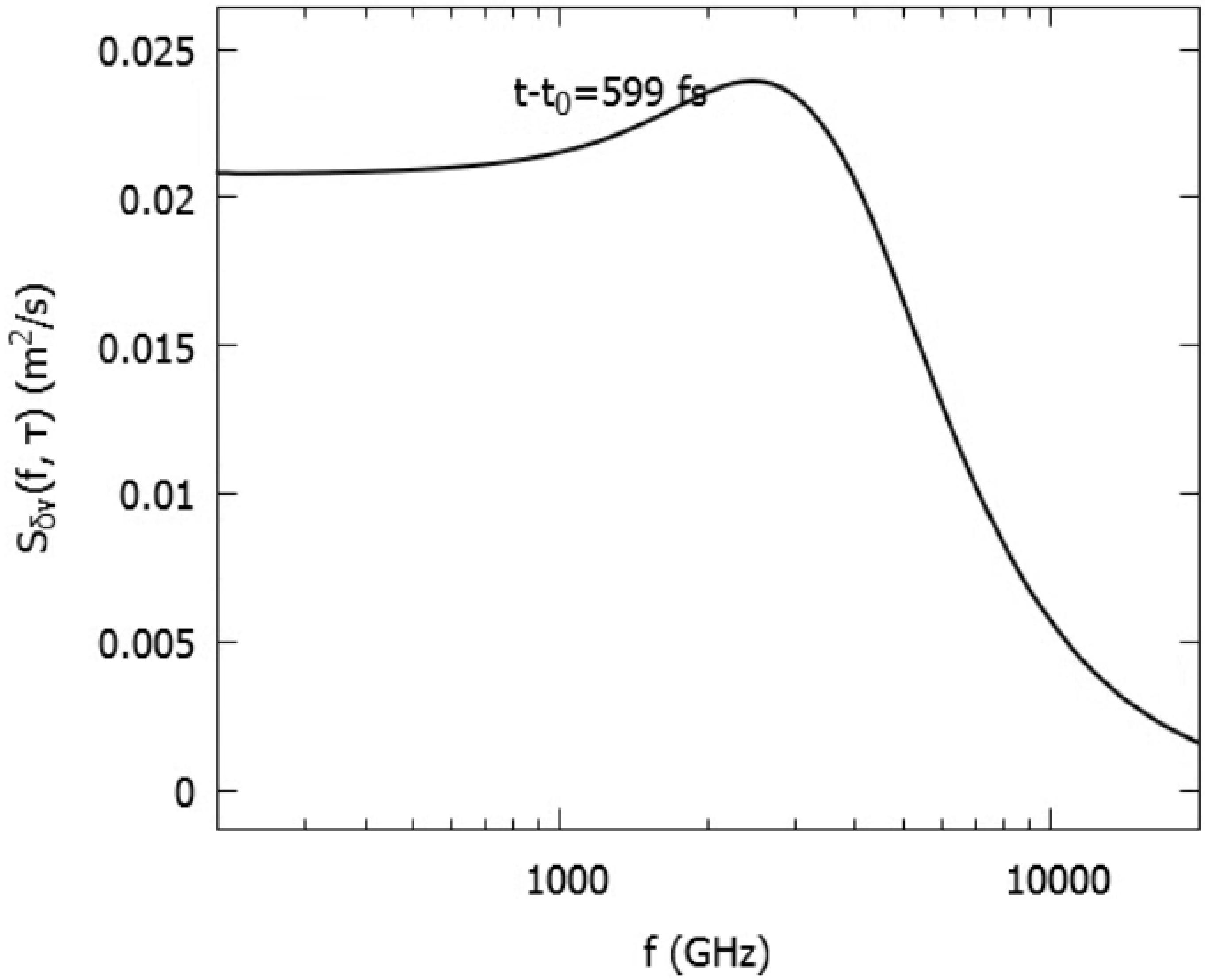

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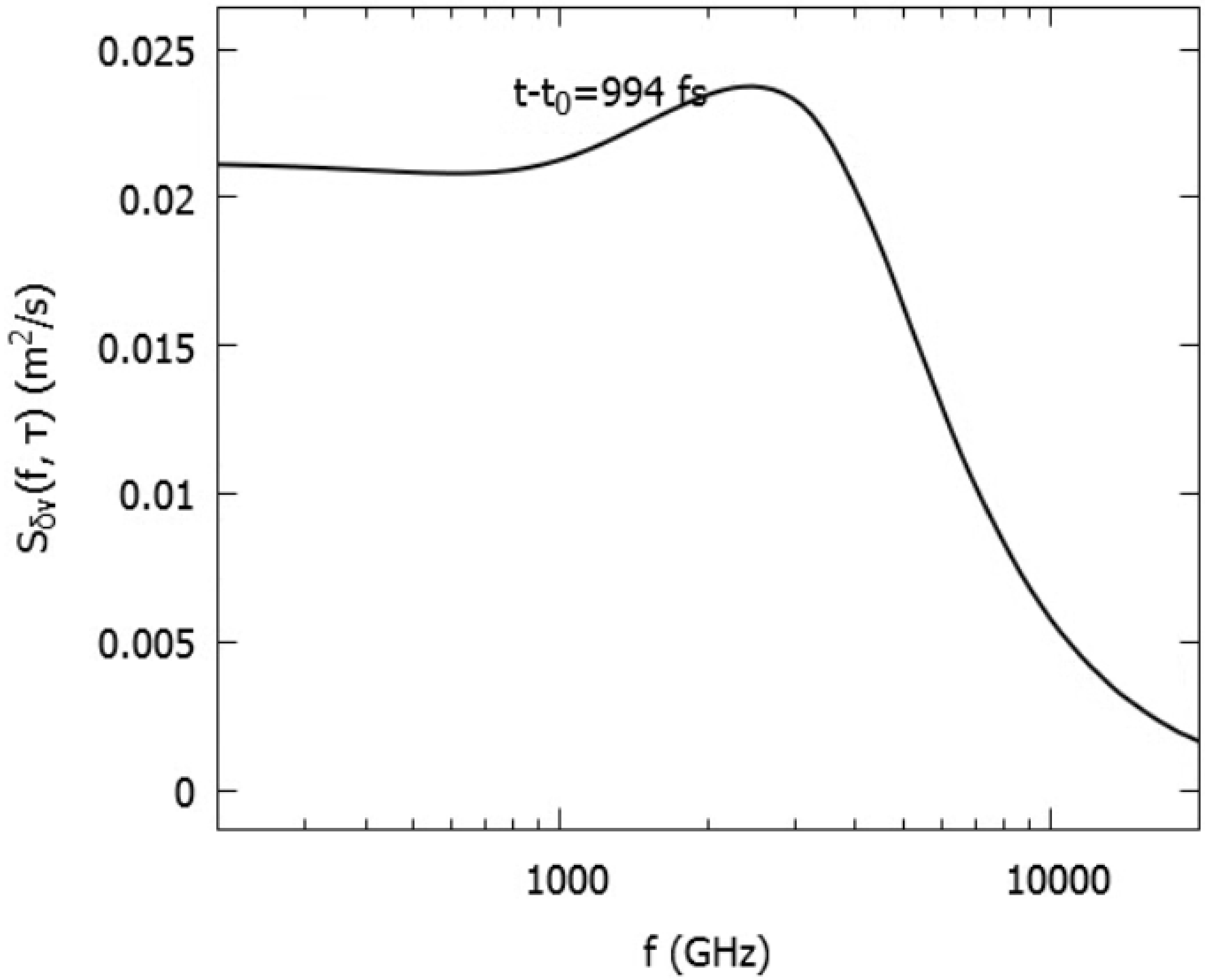
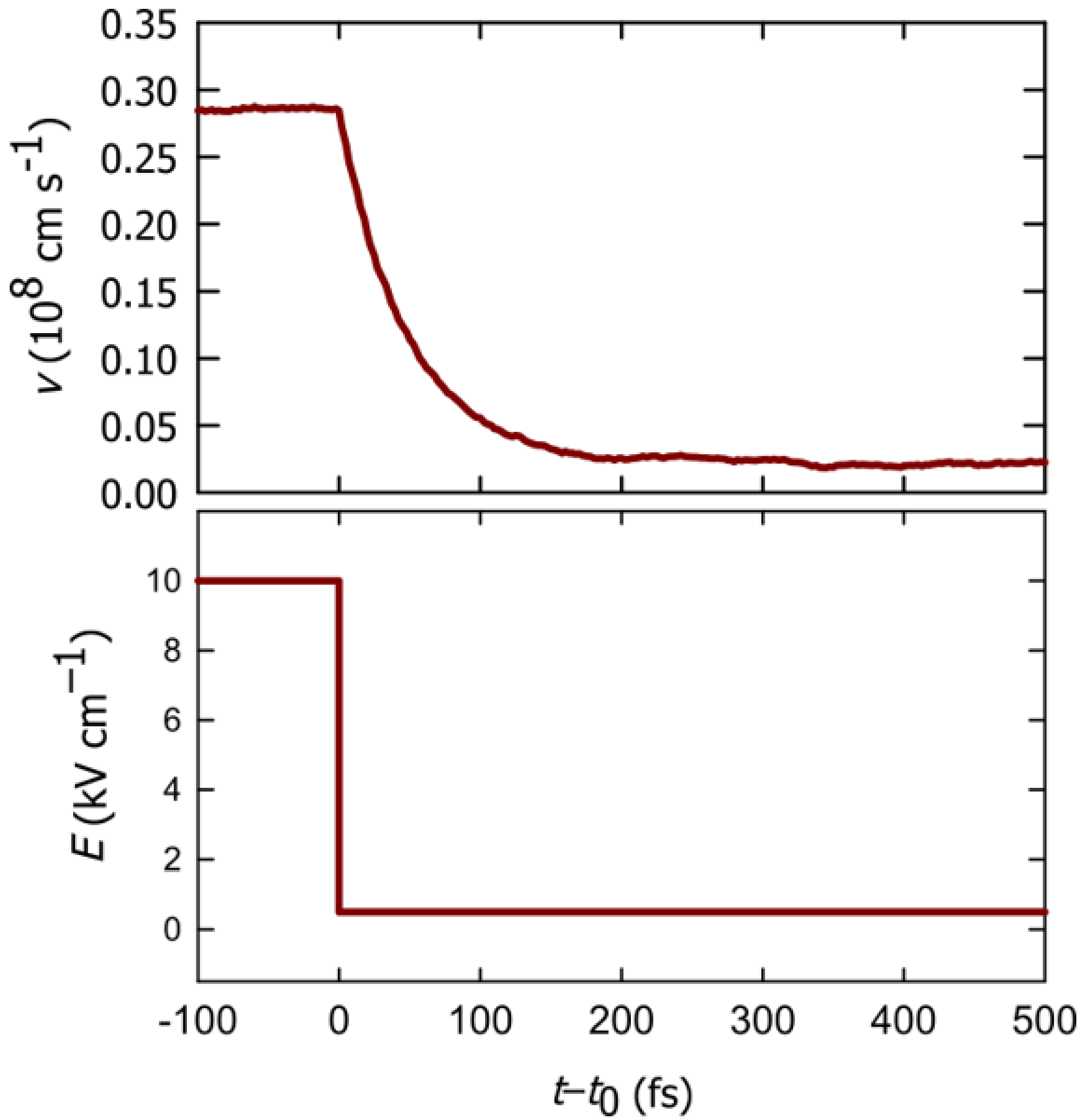
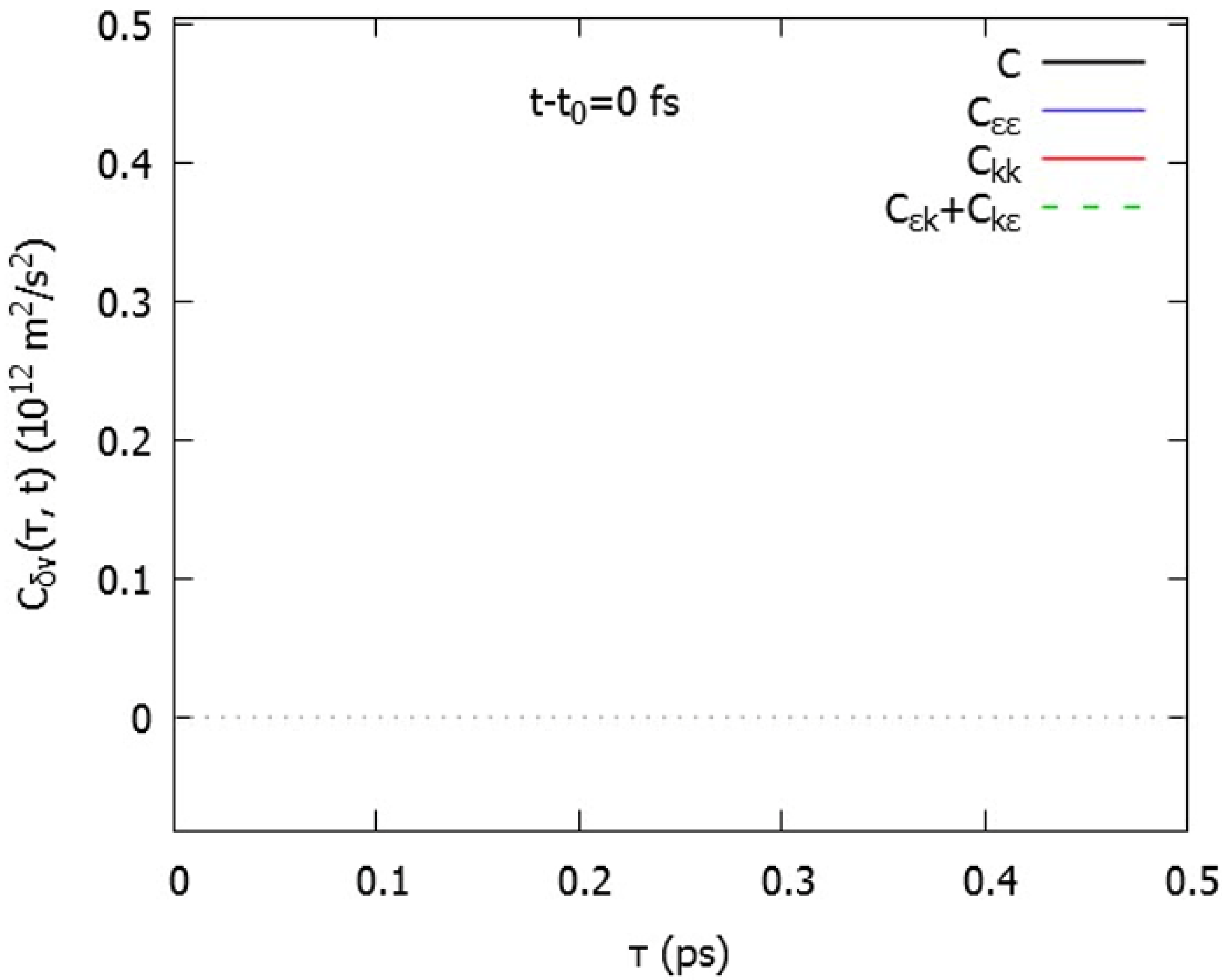


- Lorentzian shape up to 160 fs (Correlation minimum)
- Maximum starts to appear from them on at f=2200 GHz

Graphene on SiO2; **high to low** field: Transient Autocorrelation Function



Graphene on SiO2; **high to low** field: Transient Autocorrelation Function



- Strong **initial decay** of the autocorrelation at first instants due to remnant high-field energetic distribution.
- Stronger correlation at longer times indicates decreasing scattering activity.

$$C_{\varepsilon\varepsilon} = 0$$

No redistribution of the averaged velocity for the different energy levels

$$C_{kk} = C$$

A high-to-low field transient is governed by the effect of the scattering mechanisms.

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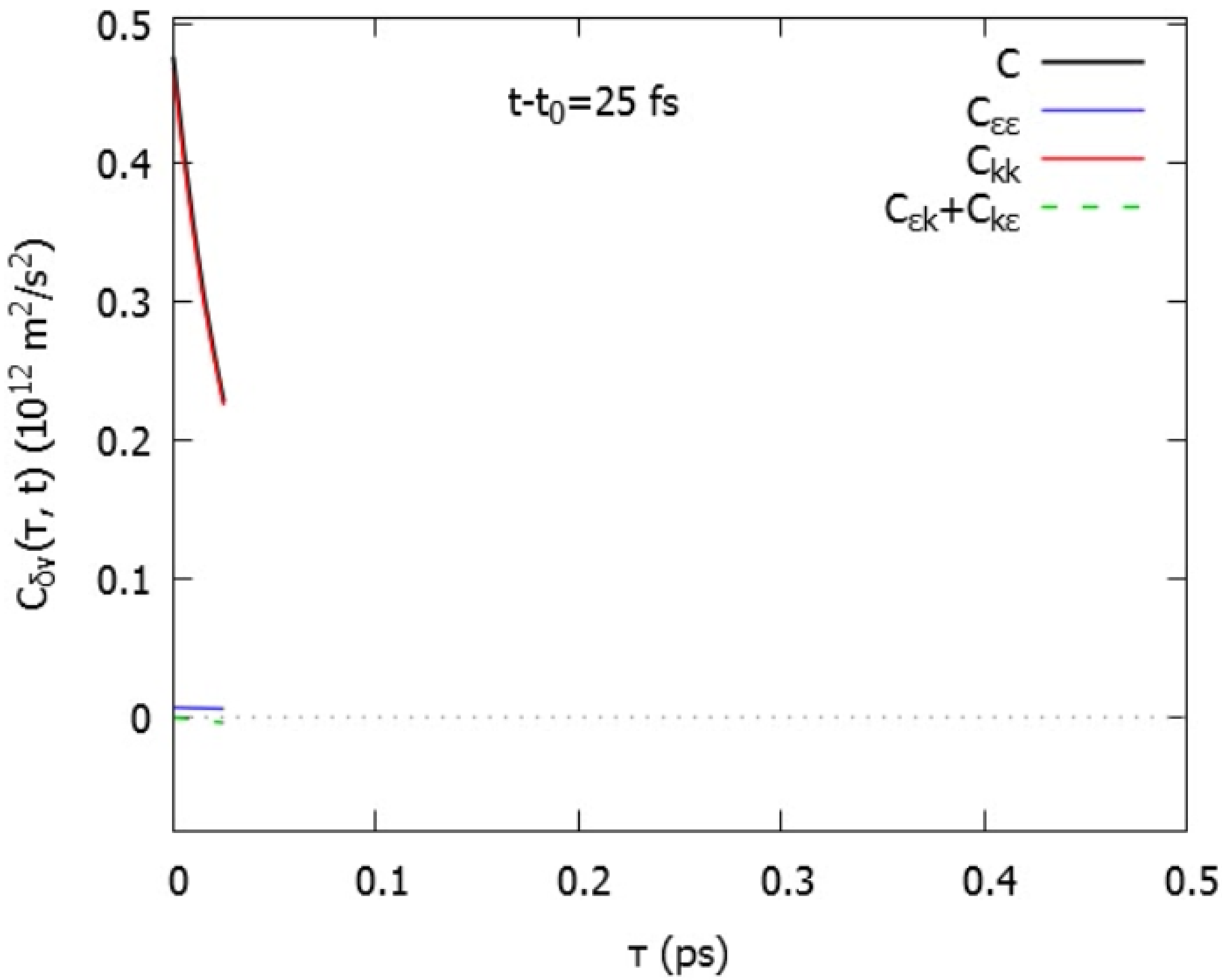

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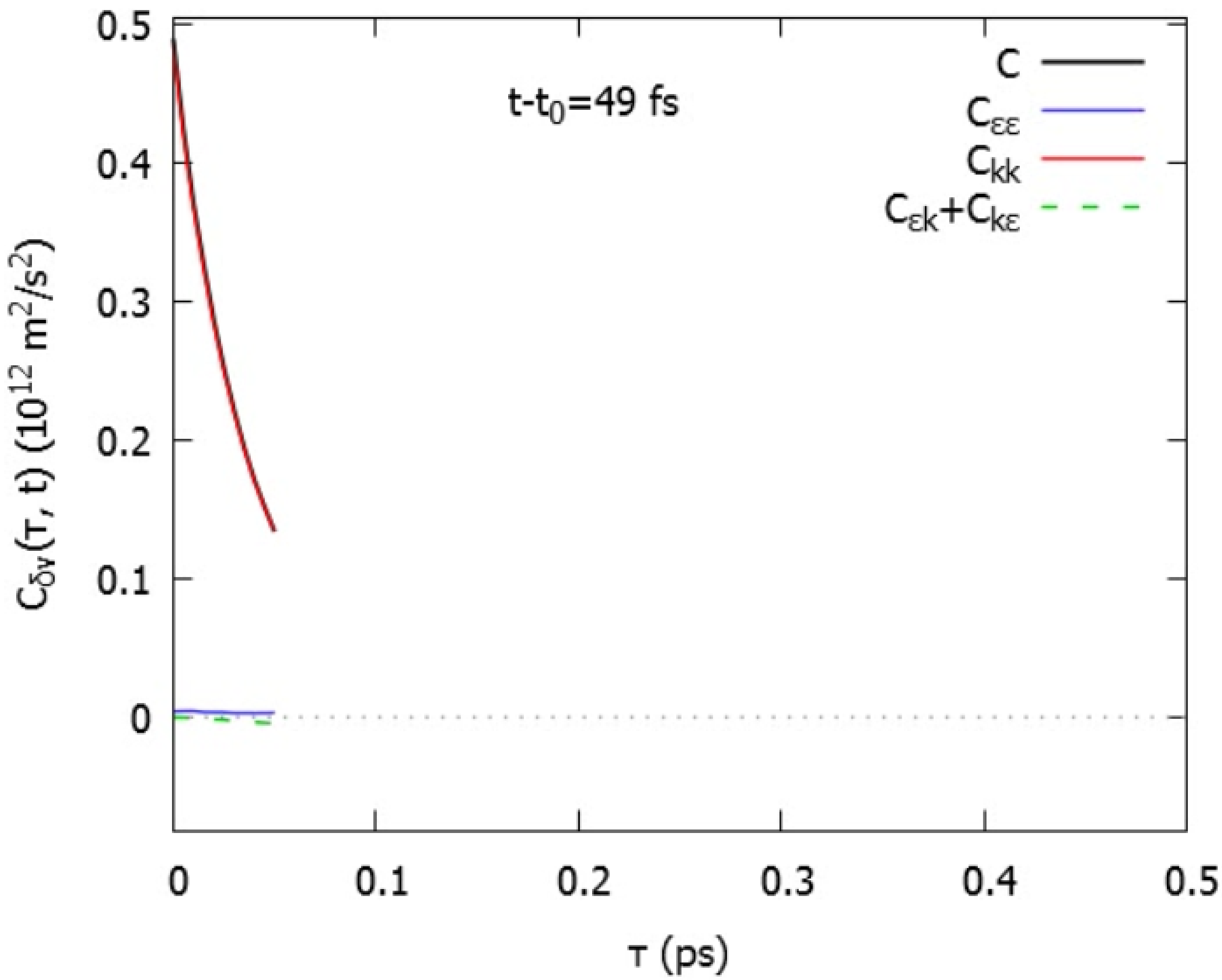

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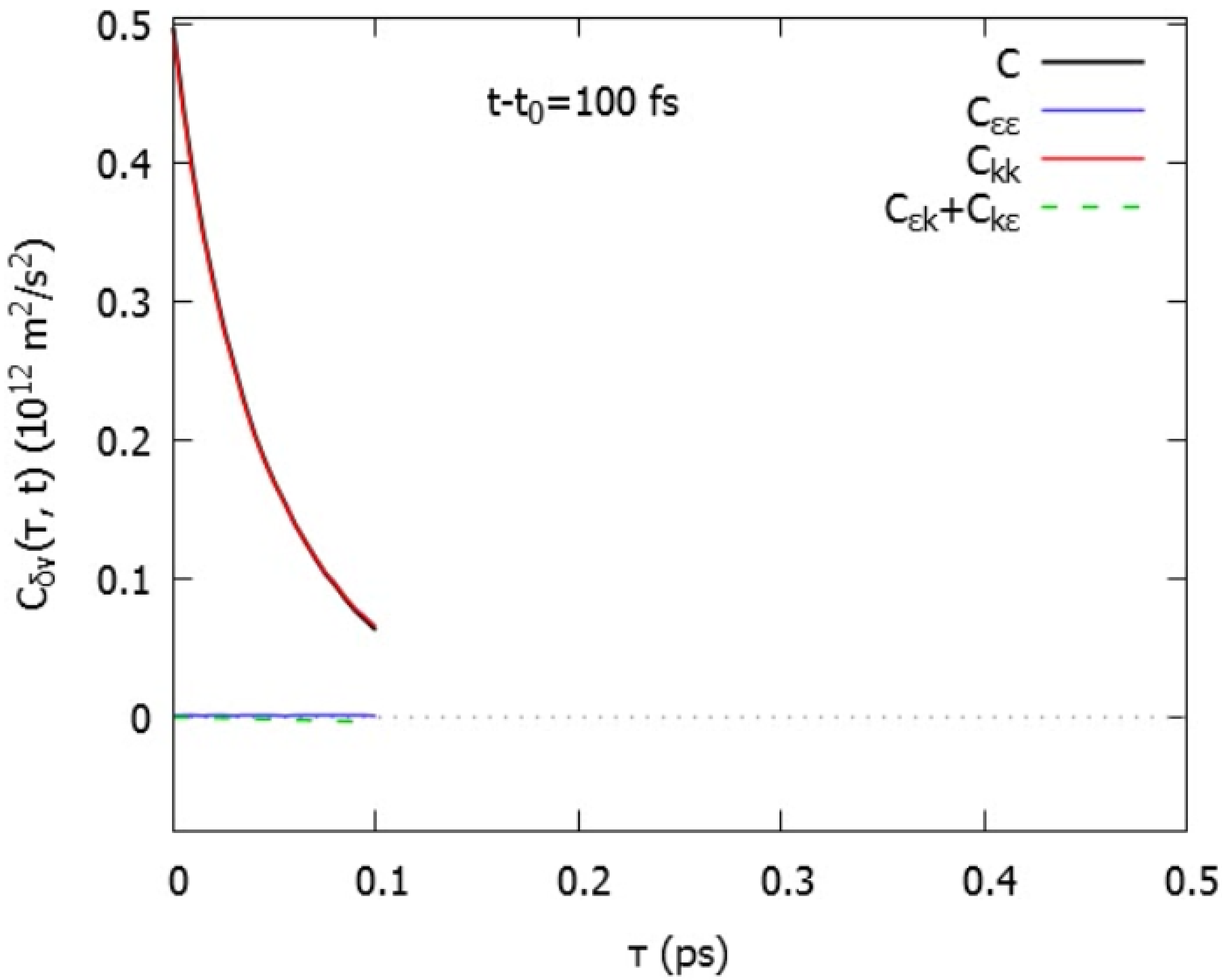

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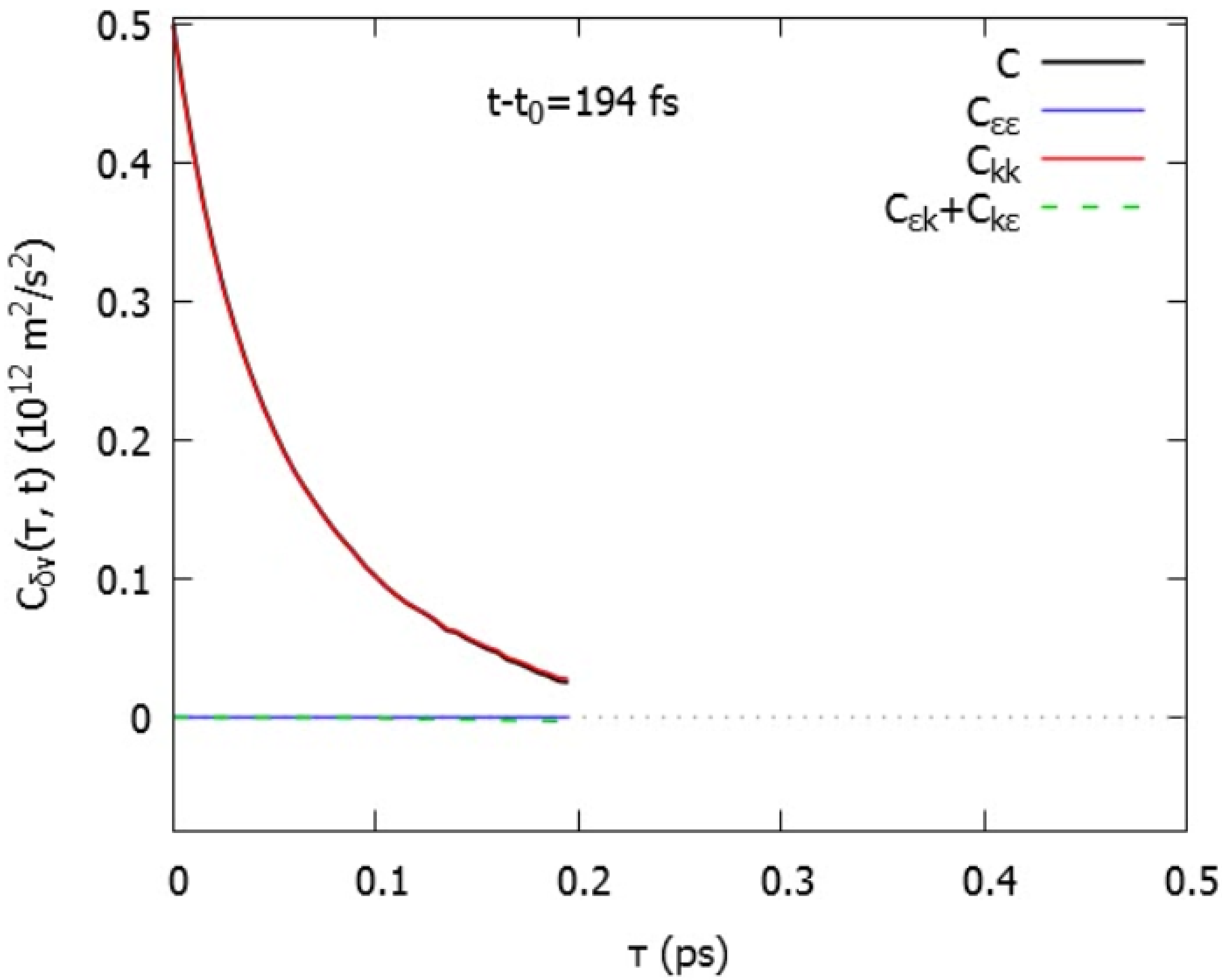

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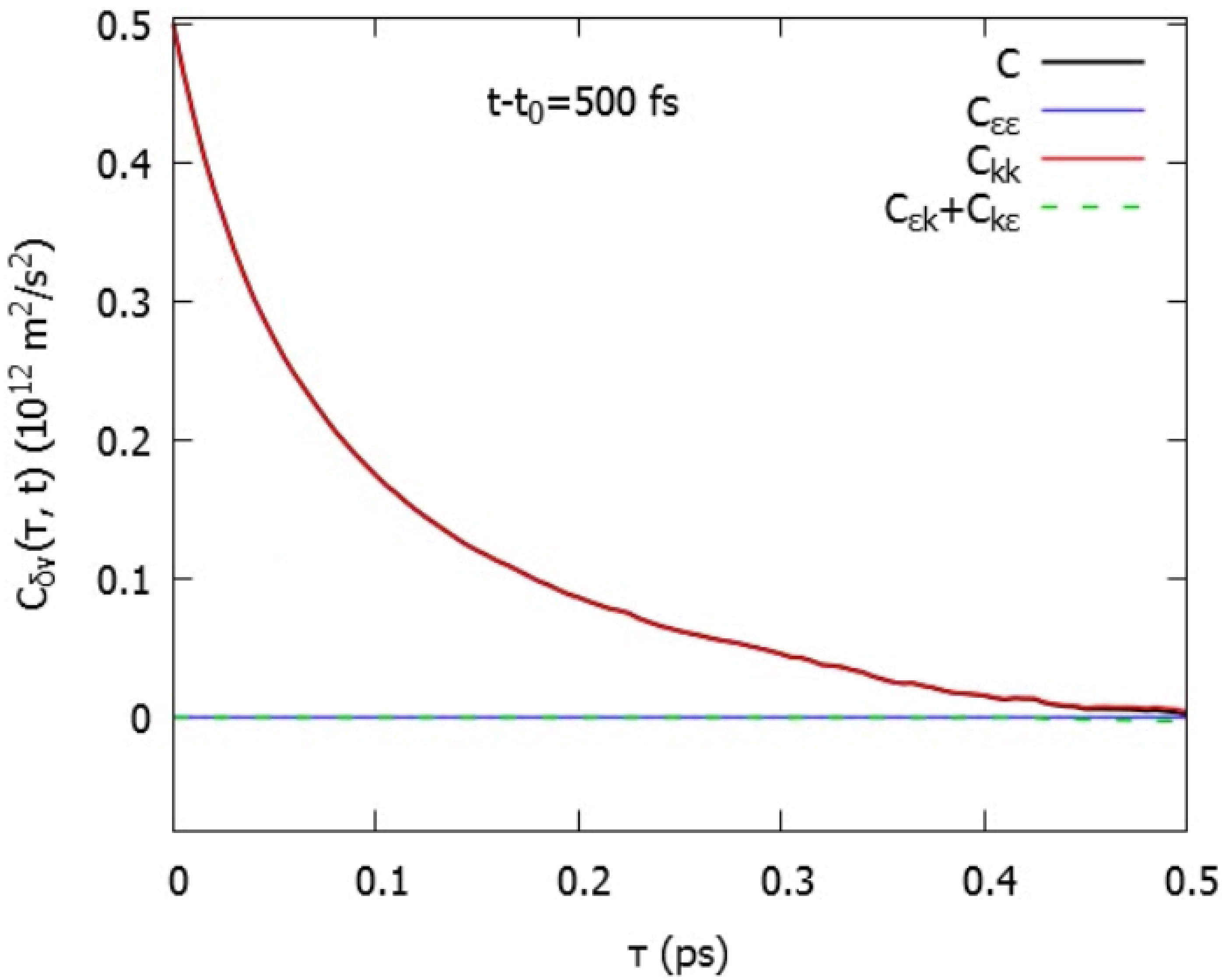

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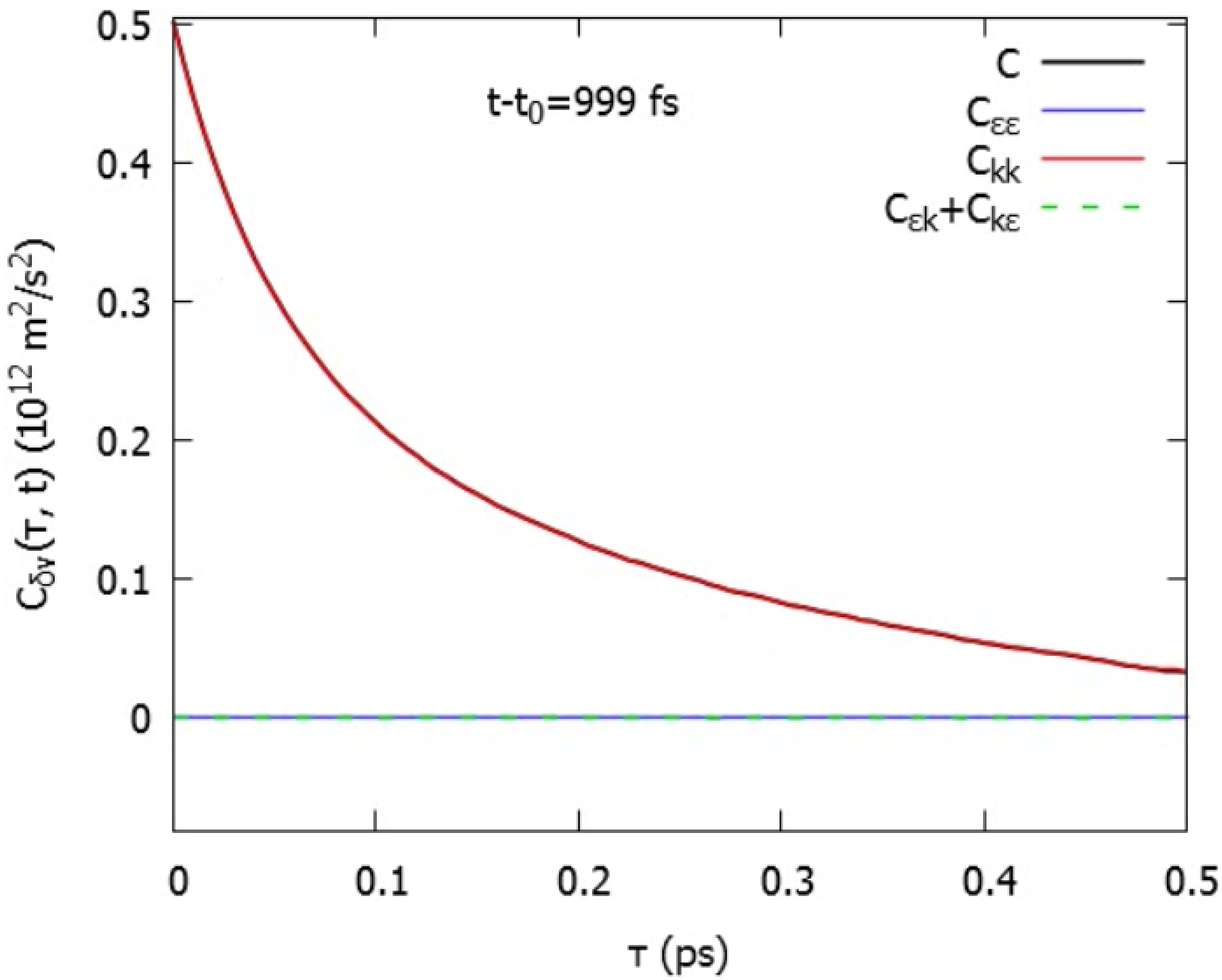

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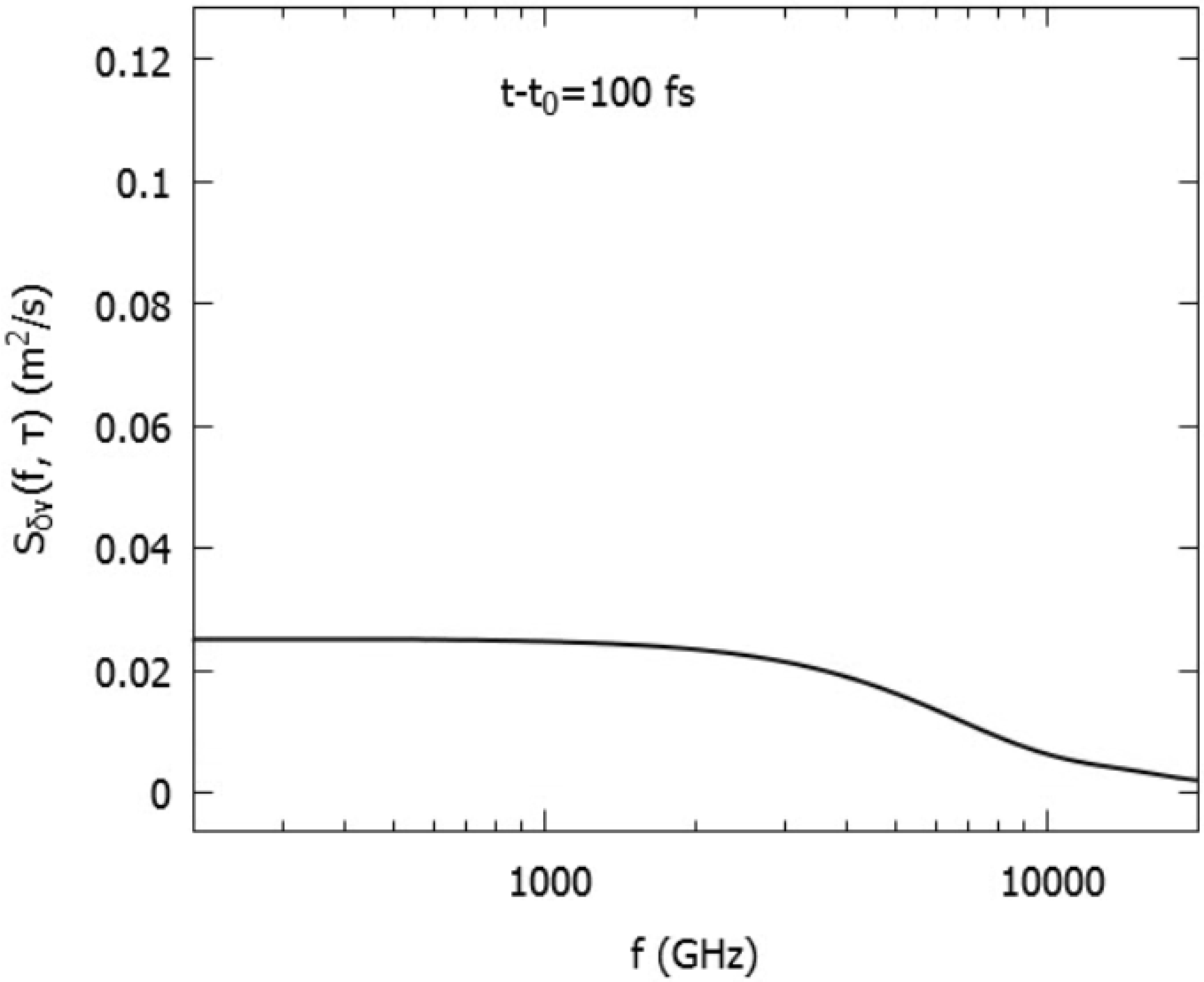
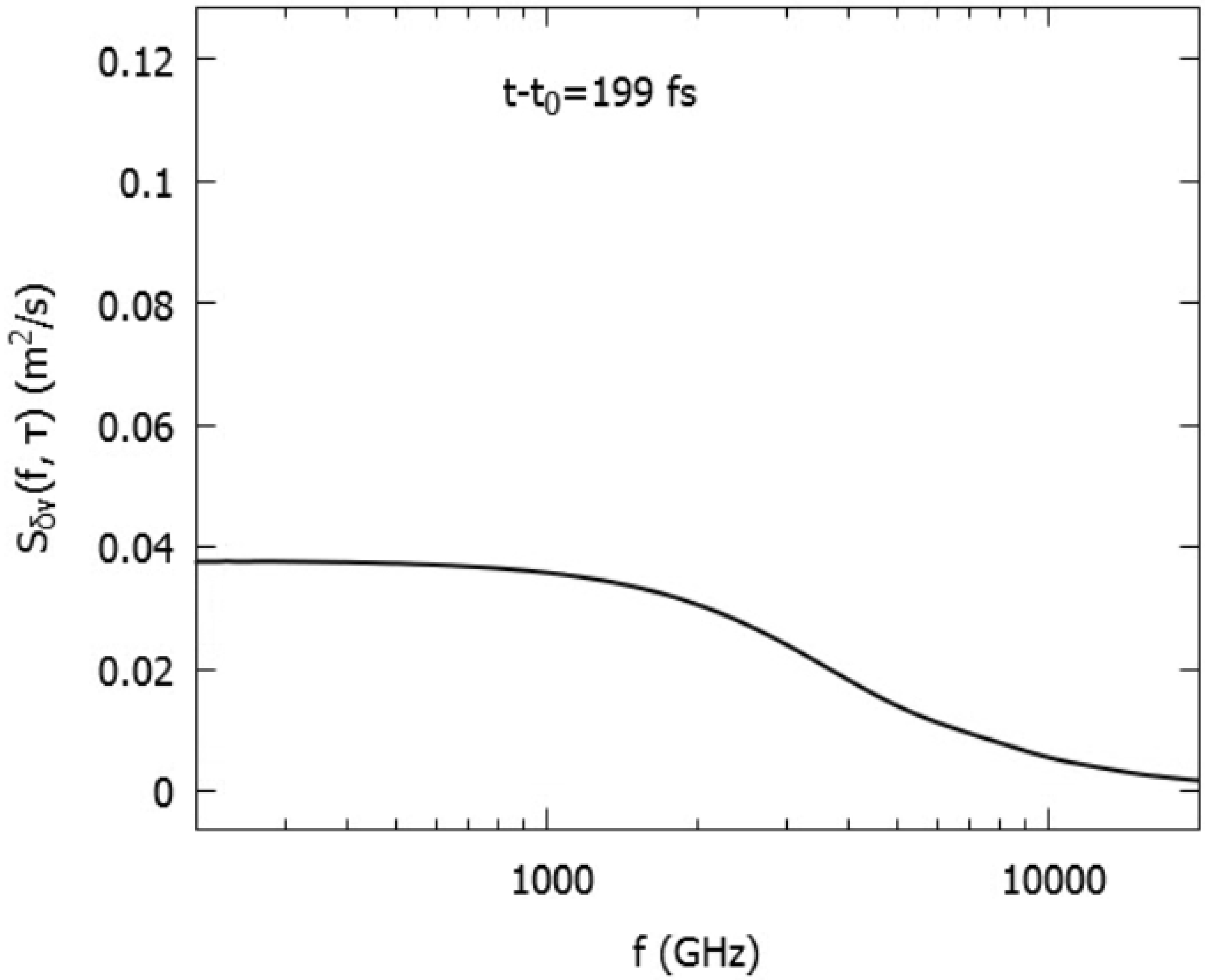
Graphene on SiO2; **high-to-low** field: Transient Power Spectral Density



- Higher Power Spectral Density as a result of longer correlation.
- No maximum appears in the sampled frequecies due to a very weak maximum at long times.

Graphene on SiO2; **high-to-low** field: Transient Power Spectral Density



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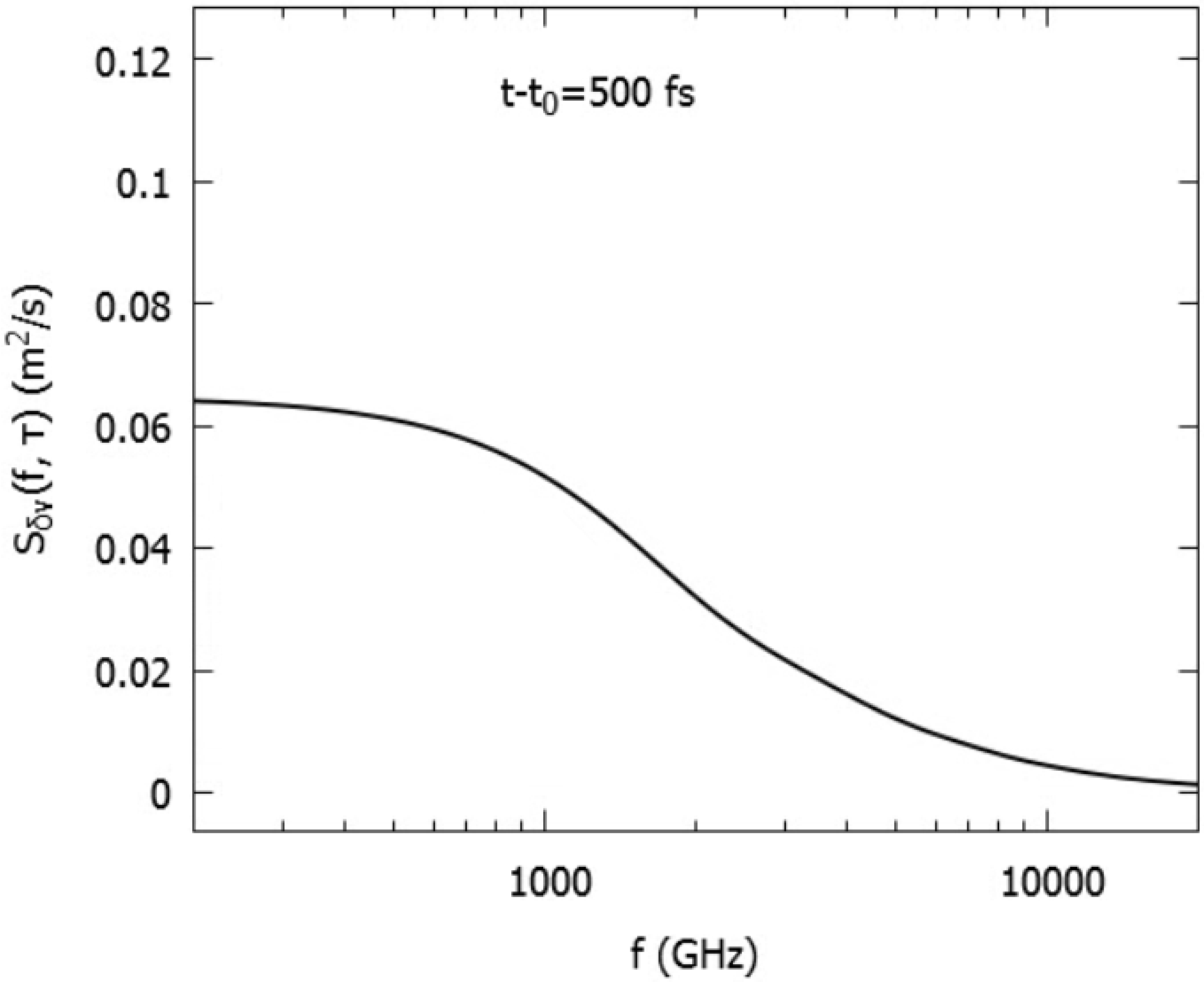

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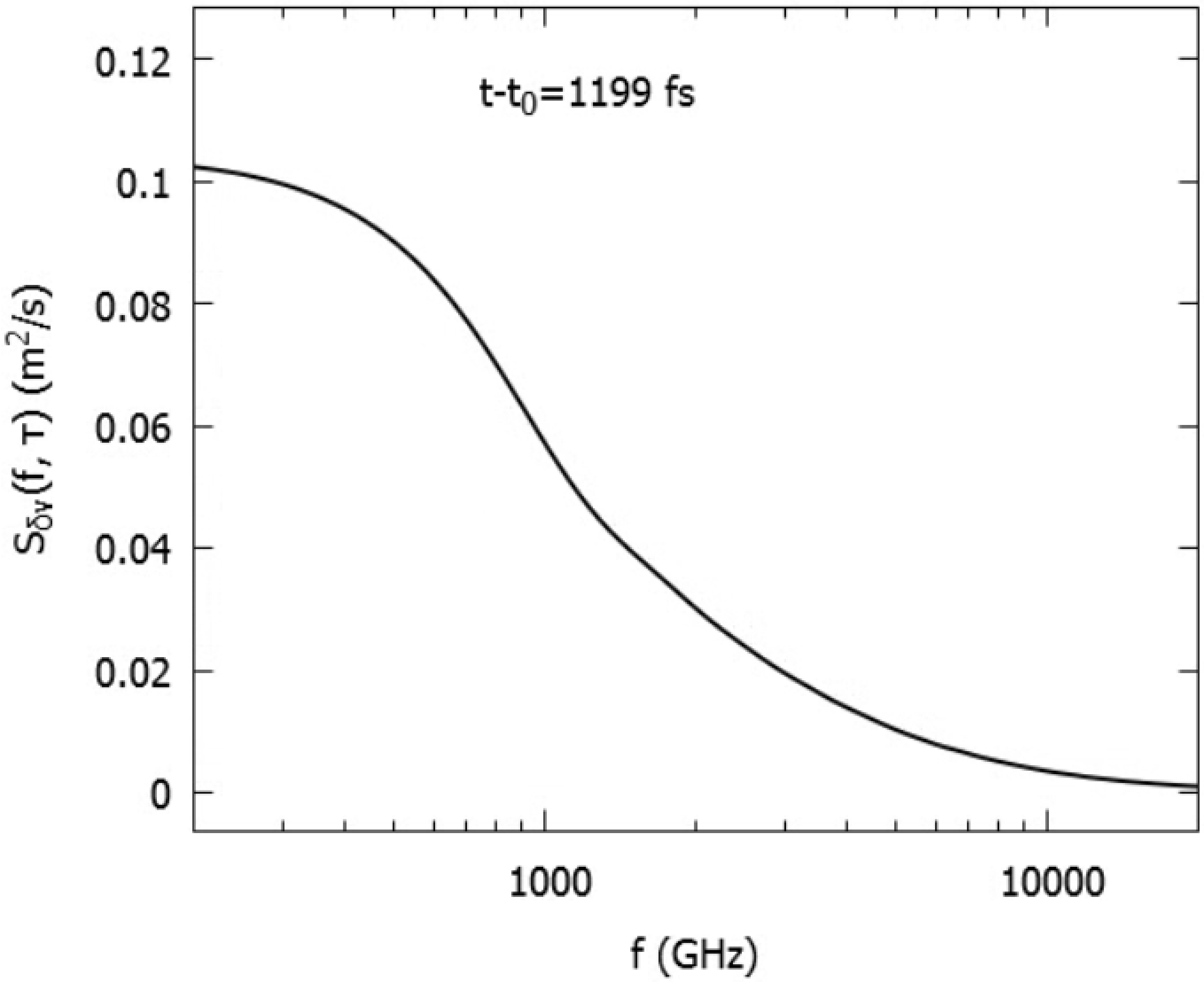

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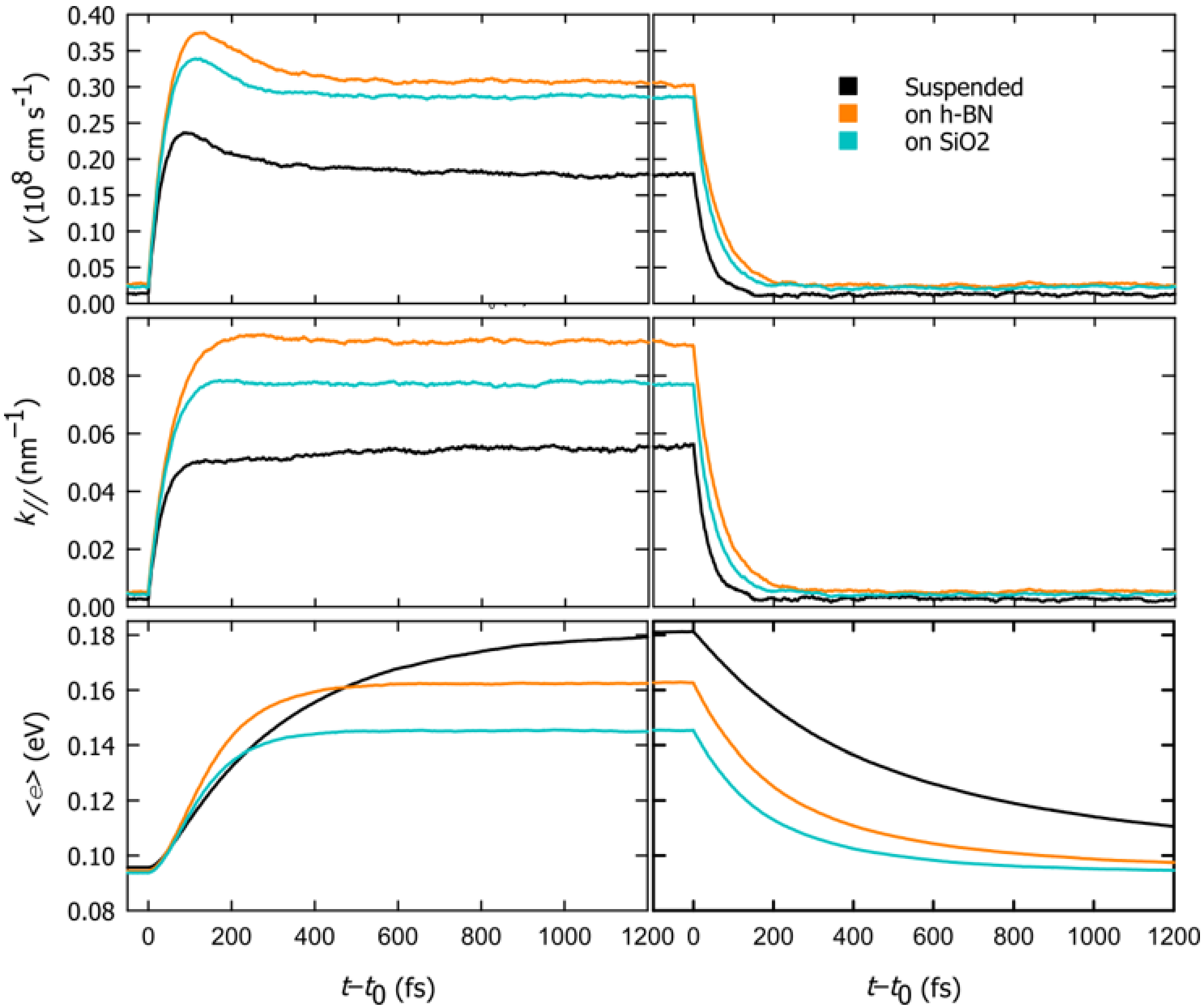
Other cases: Graphene on h-BN and Suspended graphene

Low-to-high **High-to-low**

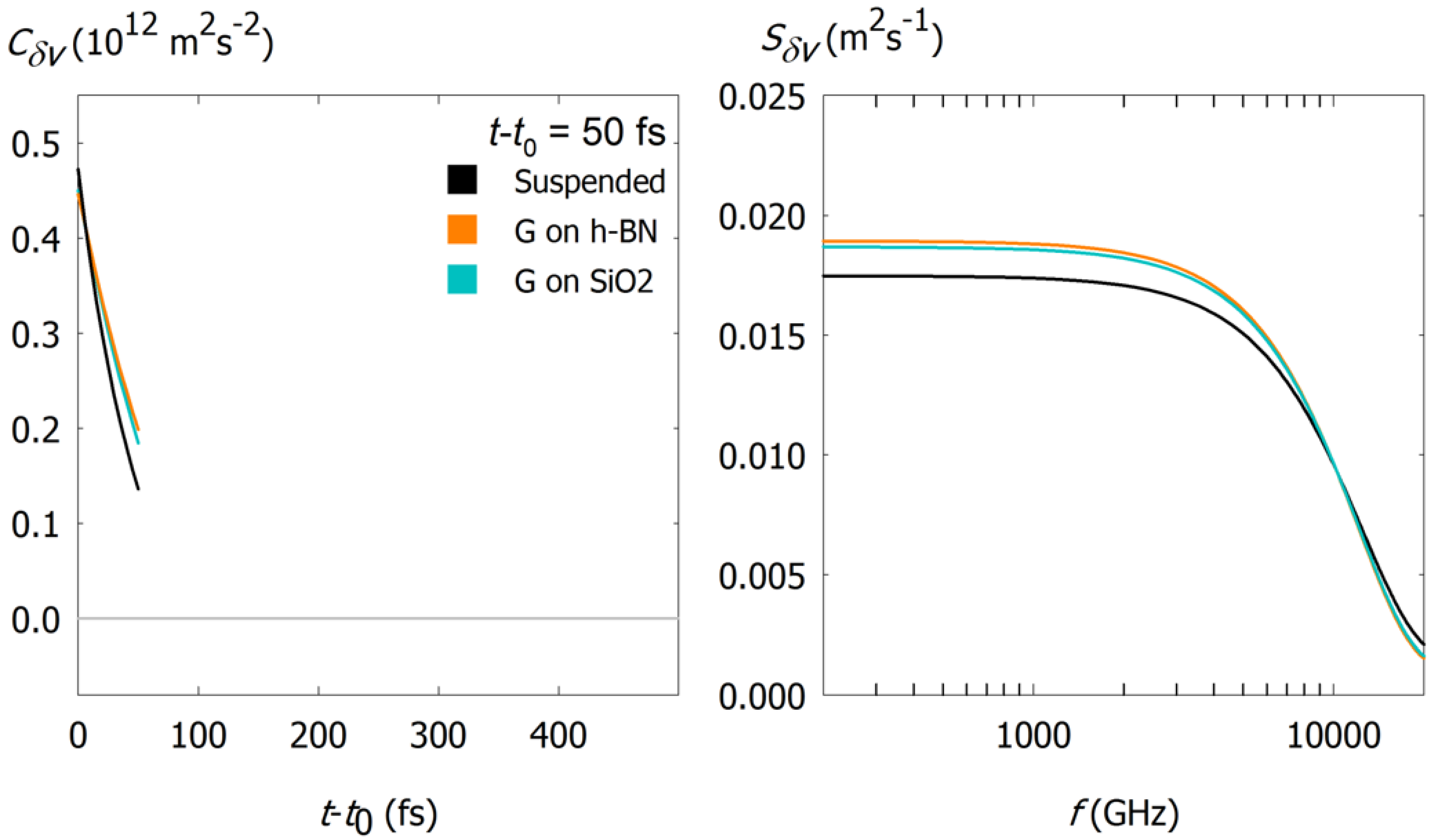


- Suspended graphene shows a faster evolutions for v and k_x but slower for the kinetic energy

Substrate Polar phonons

- Wavevector orientation

Other cases: Graphene on h-BN and Suspended graphene; **Low-to-high**



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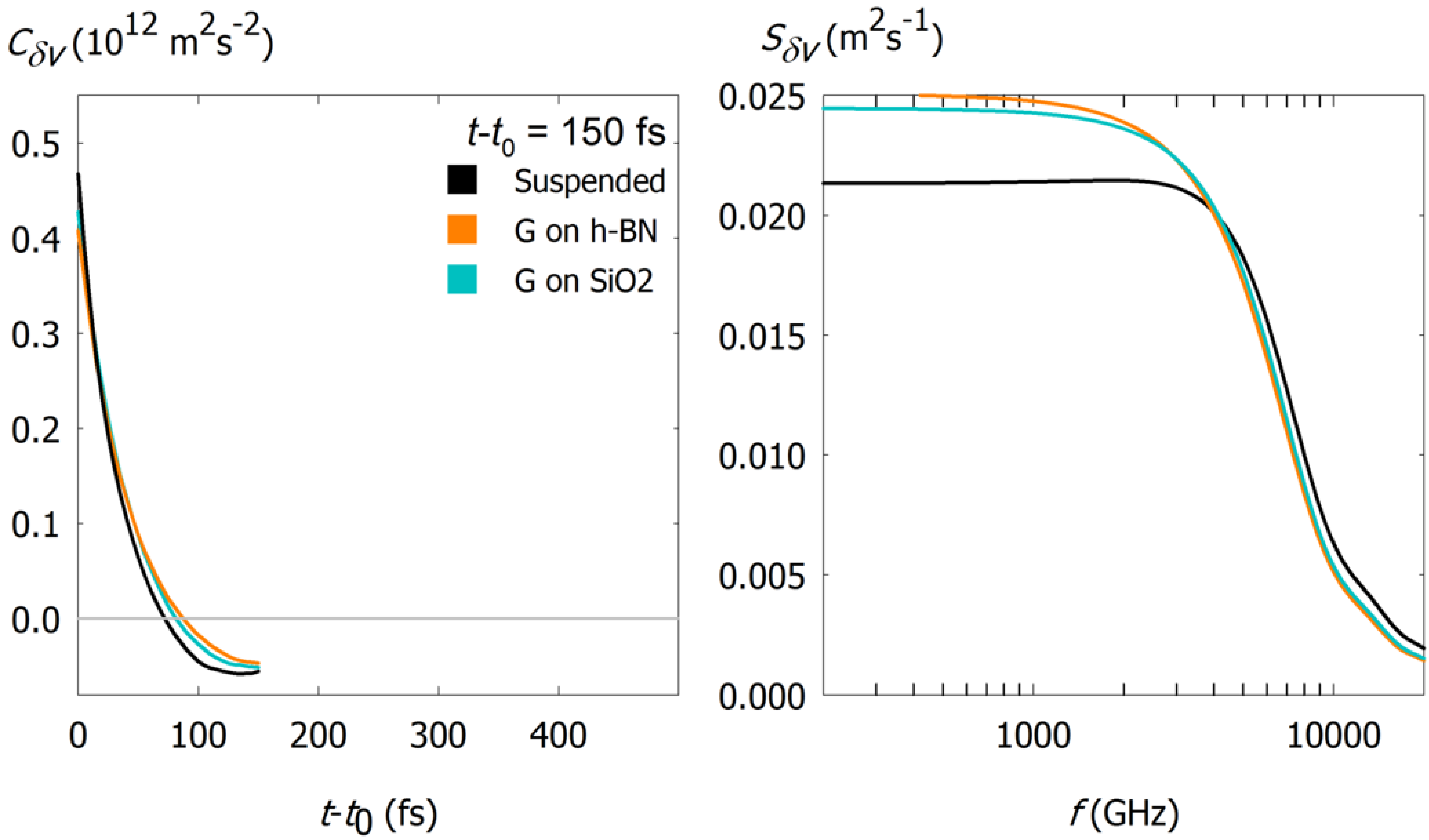

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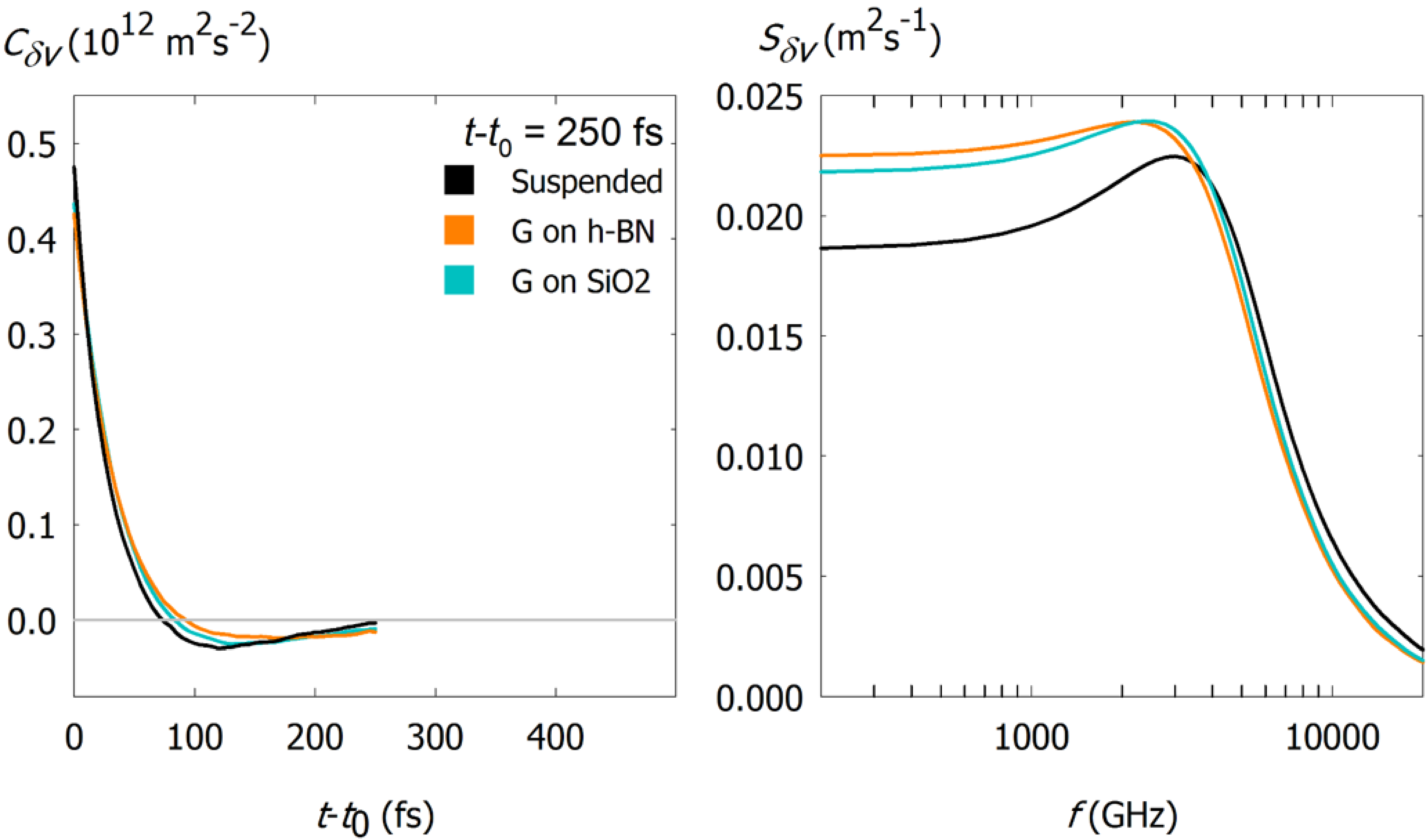

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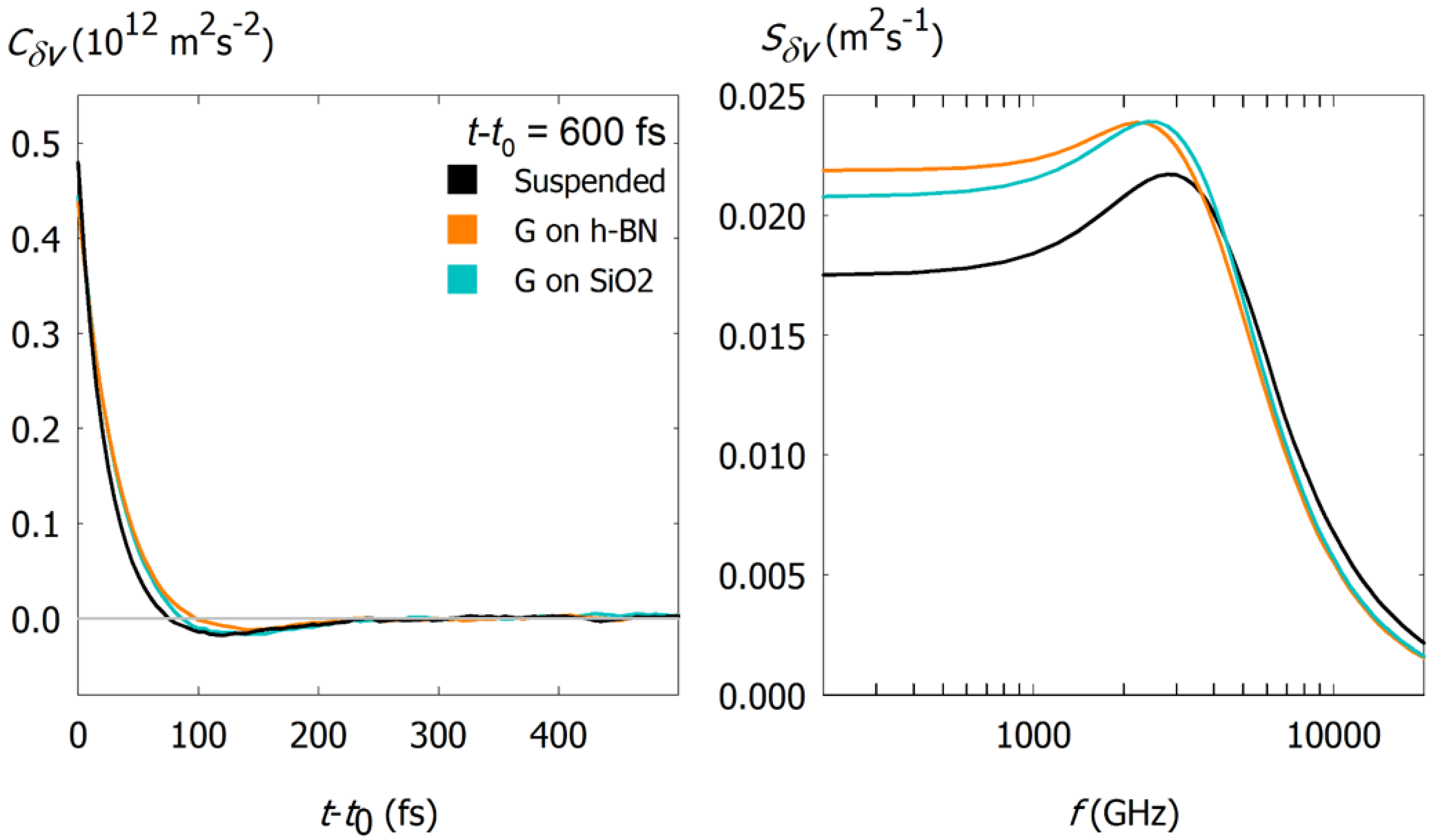
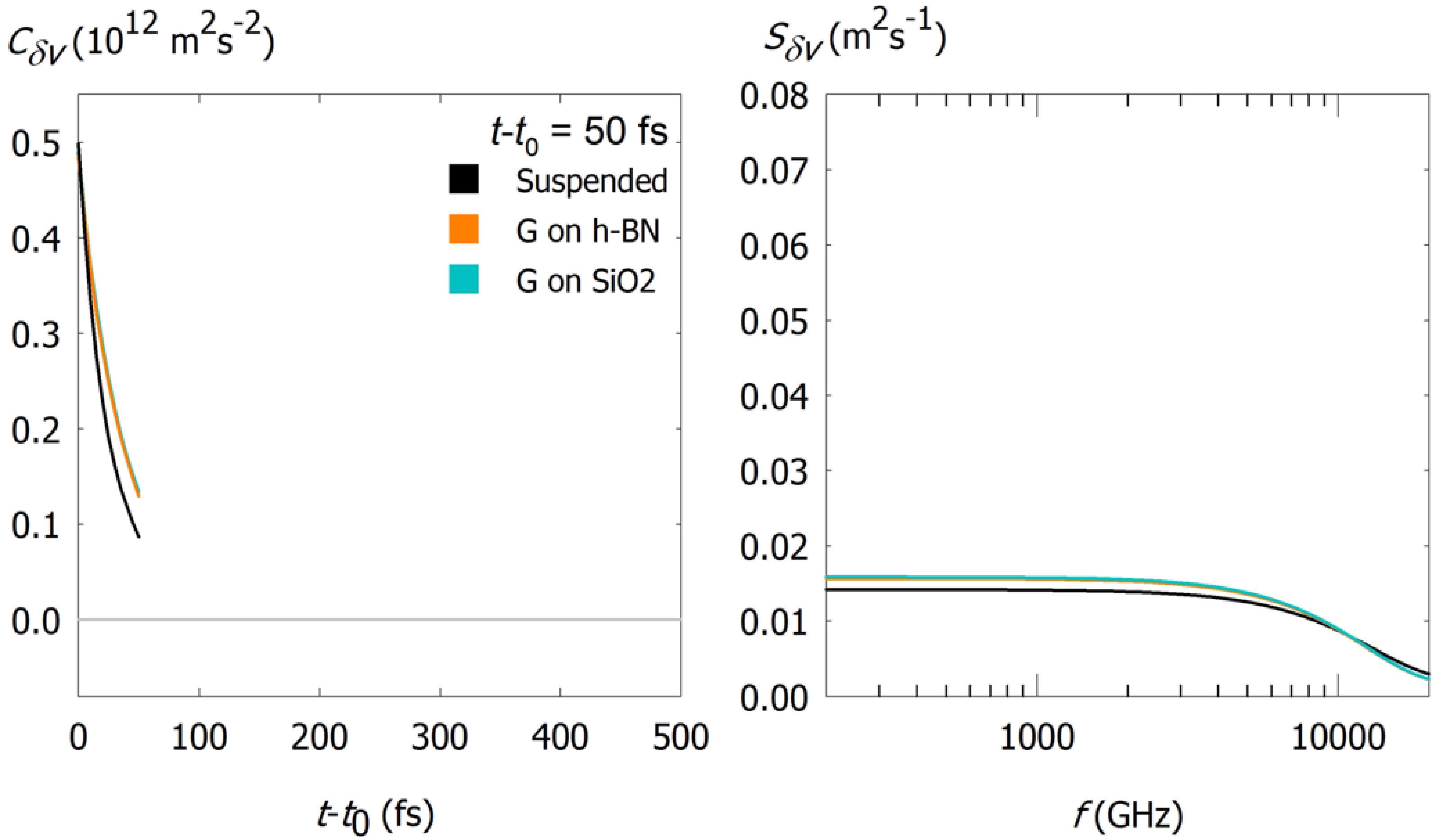


Other cases: Graphene on h-BN and Suspended graphene; **High-to-low**



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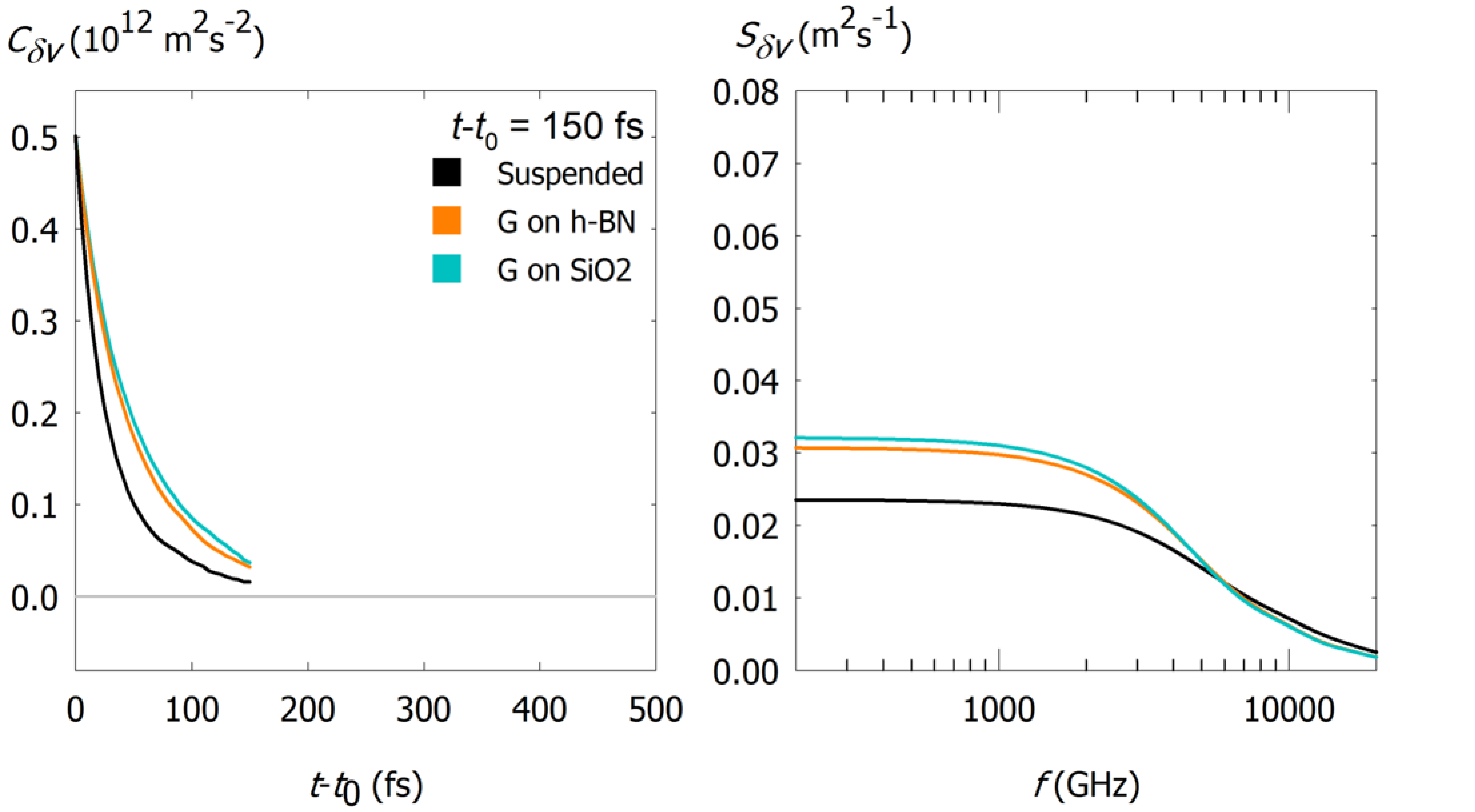

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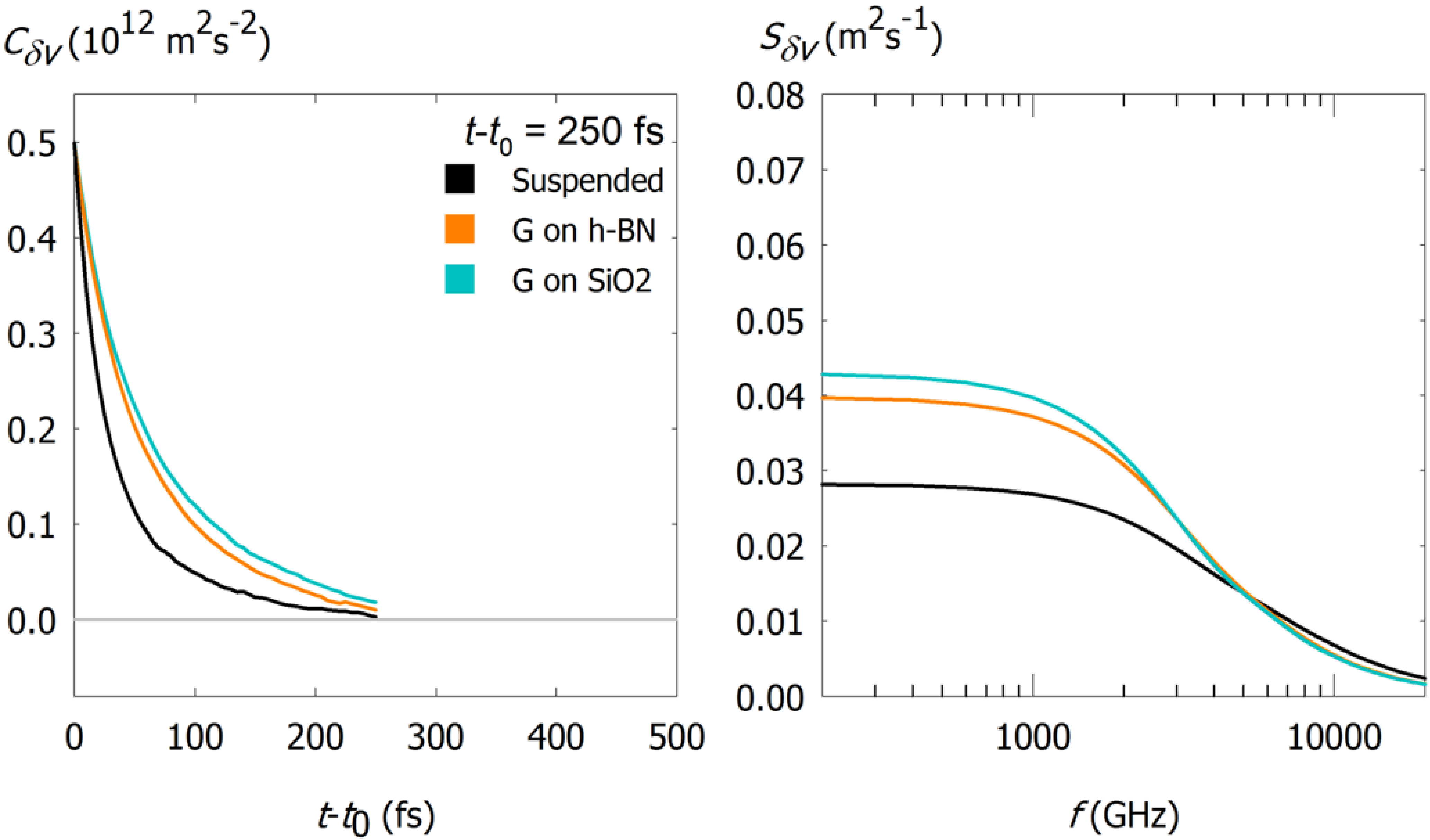

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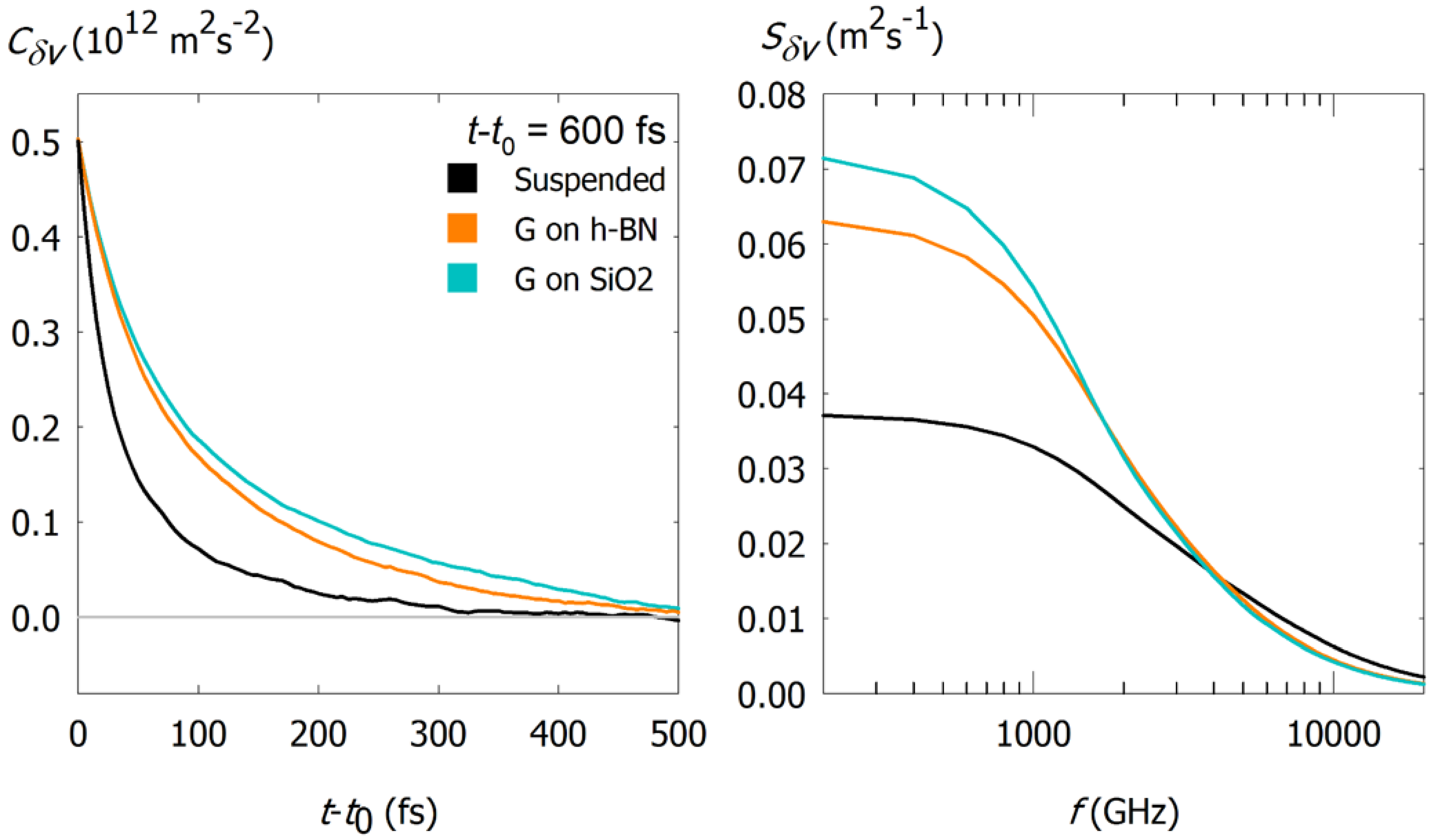

4 Conclusions

Conclusions

- Transient **velocity fluctuations** were studied with a **Monte Carlo model** for electronic transport in monolayer graphene.
- The **velocity-momentum relation in graphene** has important implications
- **Thermal contribution** to the velocity fluctuations is dominant.
- In **low-to-high field** transitions, the **convective term** becomes non negligible as a consequence of velocity overshoot
- The **substrate** presence and type is **very relevant**

Acknowledgement

This work was supported by research project **TEC2013-42622-R** from the Ministerio de Economía y Competitividad

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MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

Thanks for your attention