Rigorous Modeling of Mobilities and Relaxation Times Using Six Moments of the Distribution Function

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Outline

- Introduction
- Problems of energy-transport models
- Six moments model
- Distribution function model
- Modeling of the scattering integral
- Results
- Conclusion

Conventional Approach

- Mobilities

$$\frac{1}{n}\int \mathbf{p}\mathcal{E}^i\, Q[f]\, \mathrm{d}^3\mathbf{k} = -\left\langle \frac{\mathbf{p}\mathcal{E}^i}{\tau_p(\mathcal{E})} \right\rangle = -\mathrm{q}\,\frac{\langle \mathbf{u}\mathcal{E}^i \rangle}{\mu_i(f)}$$

- Relaxation times

$$\frac{1}{n}\int \mathcal{E}^i\, Q[f]\, \mathrm{d}^3\mathbf{k} = -\left\langle \frac{\mathcal{E}^i}{\tau_{\mathcal{E}^i}(\mathcal{E})} \right\rangle = -\frac{\langle \mathcal{E}^i \rangle - \langle \mathcal{E}^i \rangle_{\mathrm{eq}}}{\tau_i(f)}$$

- Relaxation time approximation

$$\mu_i(f) \approx \mu_i(\langle \mathcal{E} \rangle) \qquad \text{and} \qquad \tau_i(f) \approx \tau_i(\langle \mathcal{E} \rangle)$$

- Common assumptions

$$\mu_1 = \mu_0 \qquad \text{and} \qquad \tau_1 = \mathrm{const}$$

Energy-Transport Model

- First four moments of BTE
- Highest order moment $\langle \mathcal{E}^2 \rangle$

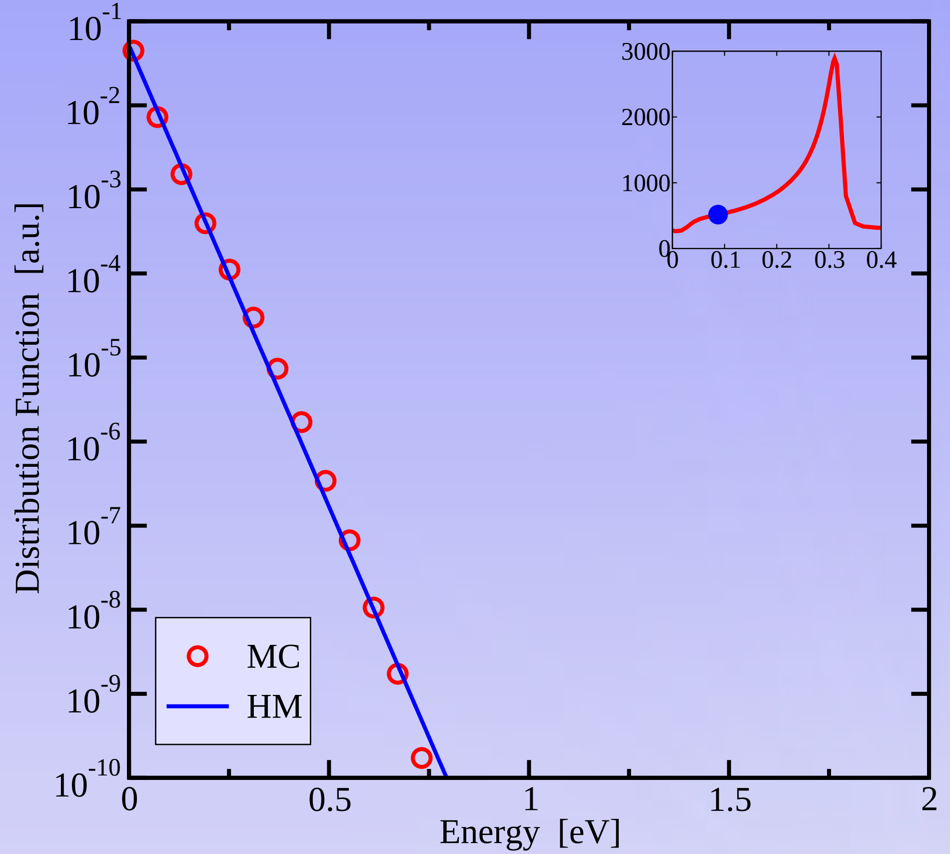
$$\langle \mathcal{E}^2 \rangle = \frac{5}{3} \langle \mathcal{E} \rangle^2$$

- Heated Maxwellian DF

$$f(\mathcal{E}) = A \exp\left(-\frac{\mathcal{E}}{\mathrm{k_B} T_n}\right)$$

Single valued function

Hot carriers overestimated



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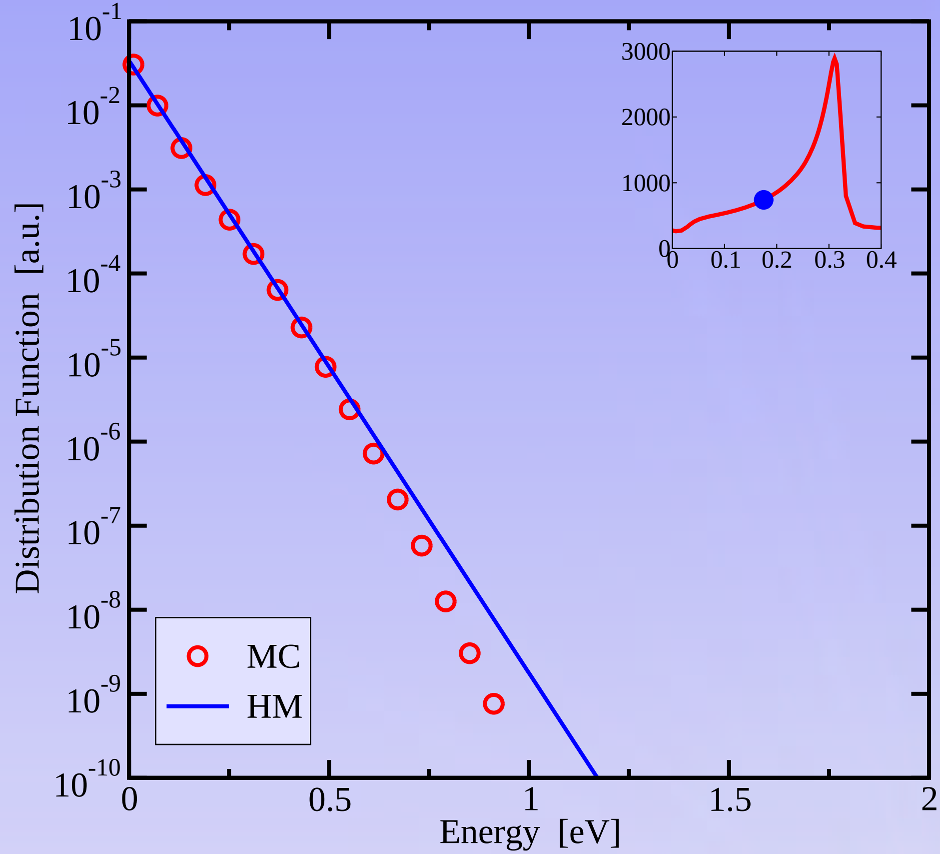

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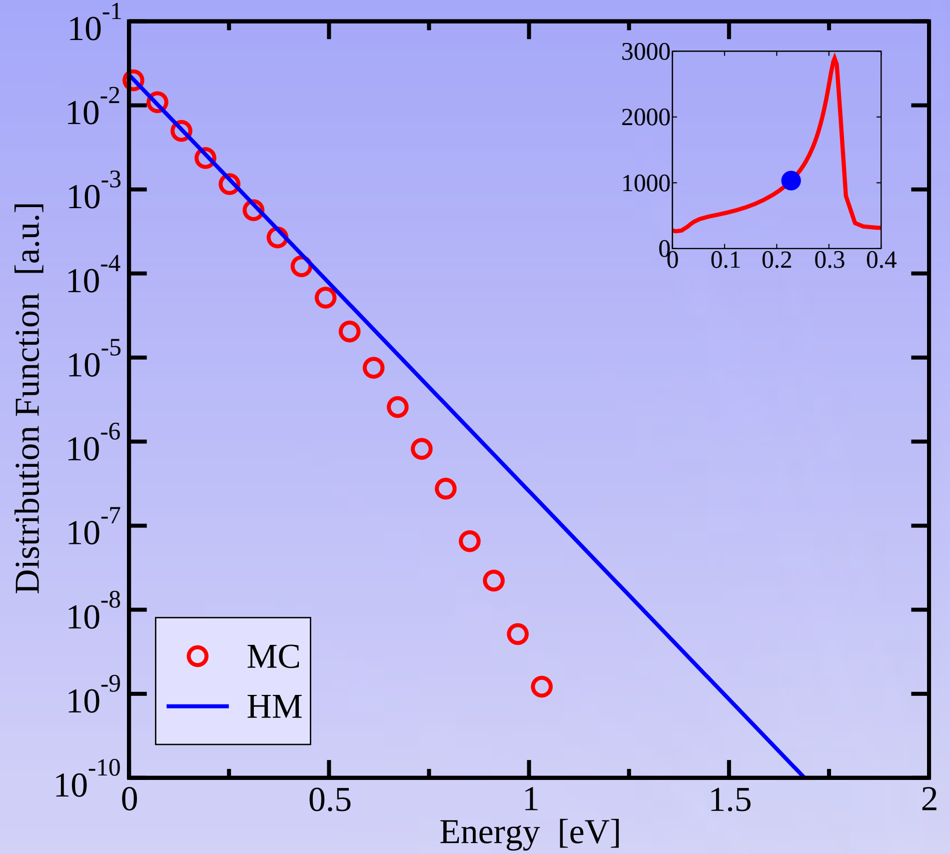

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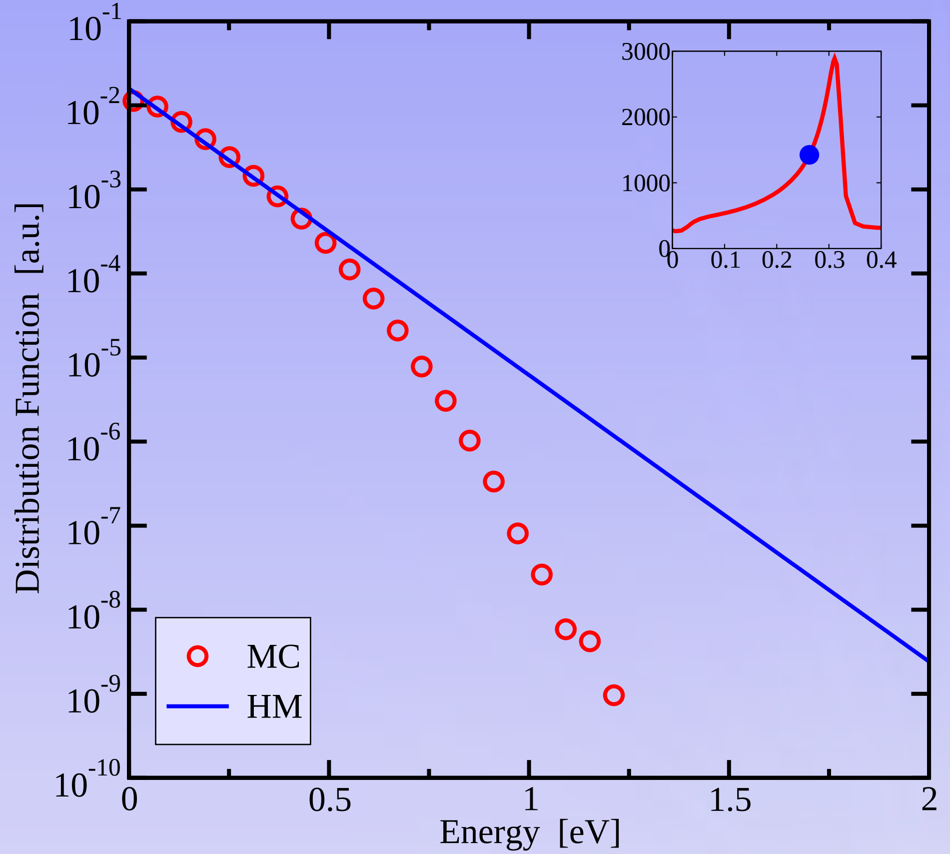

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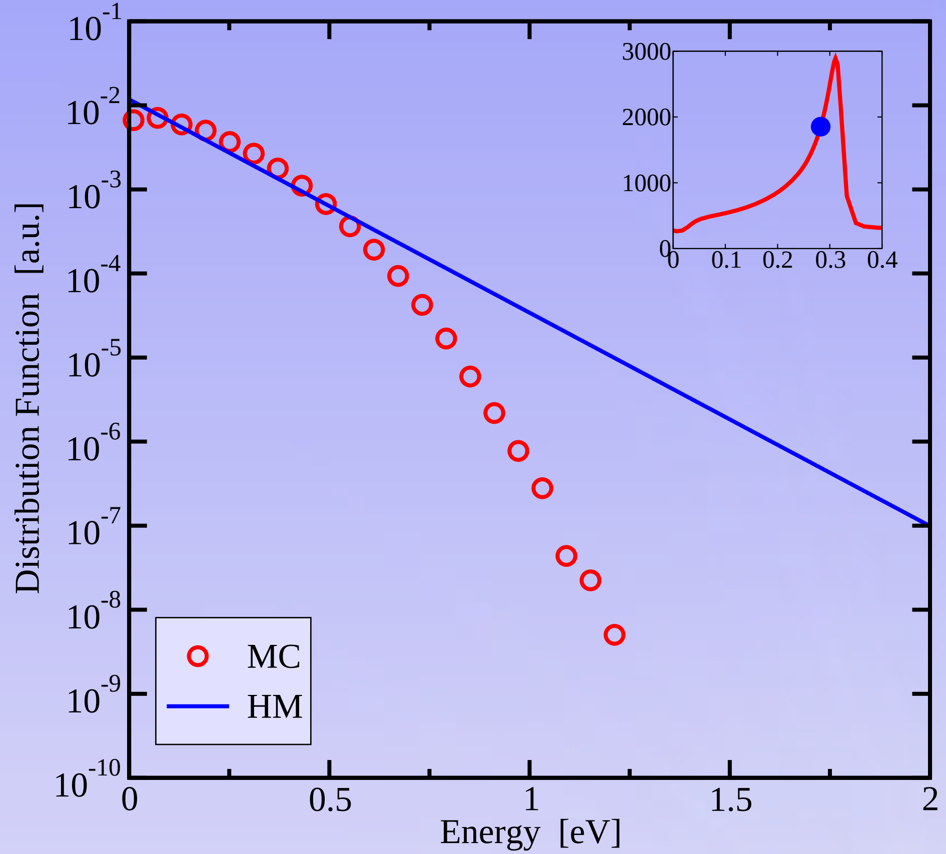

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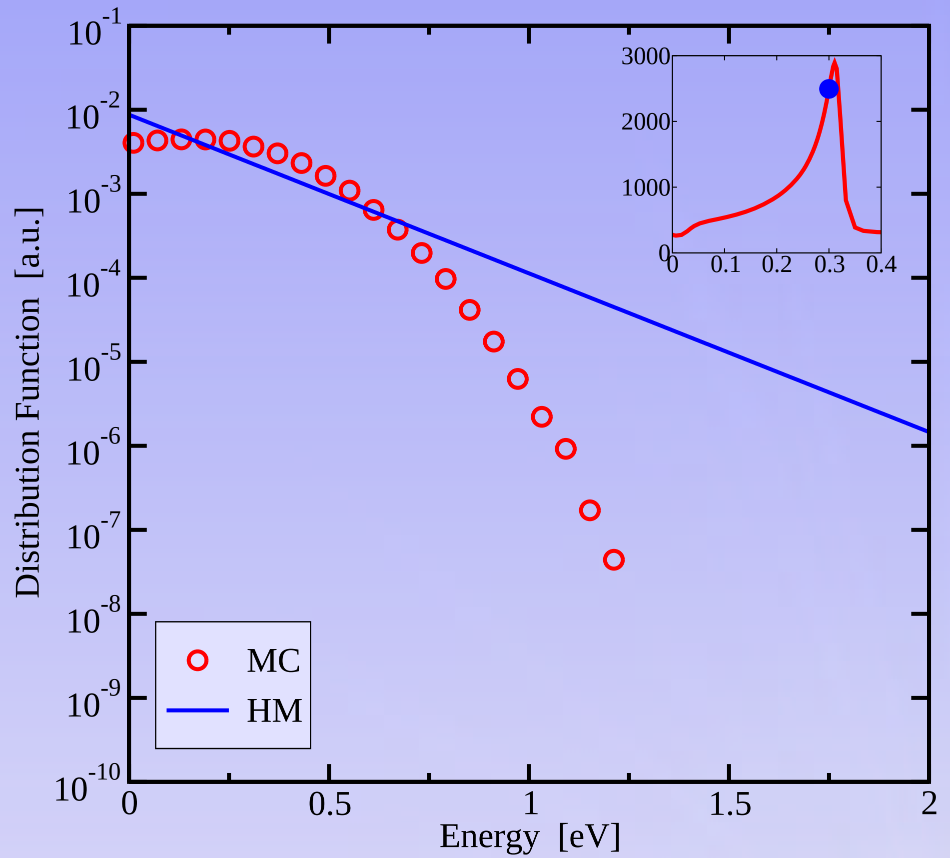

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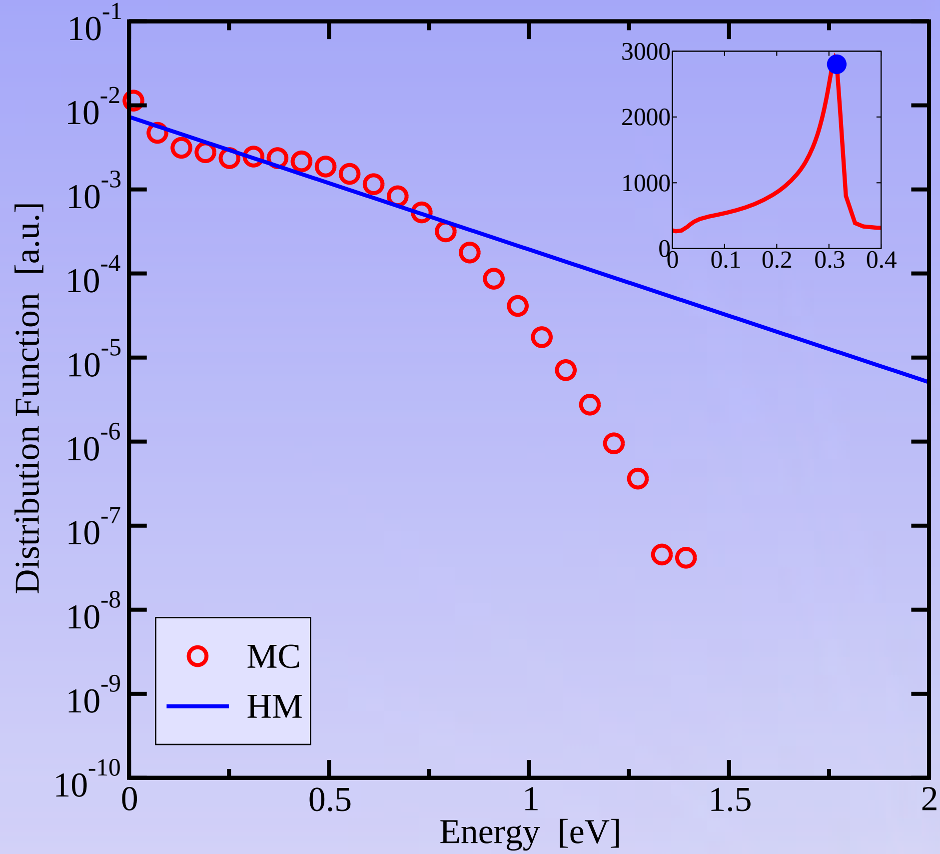

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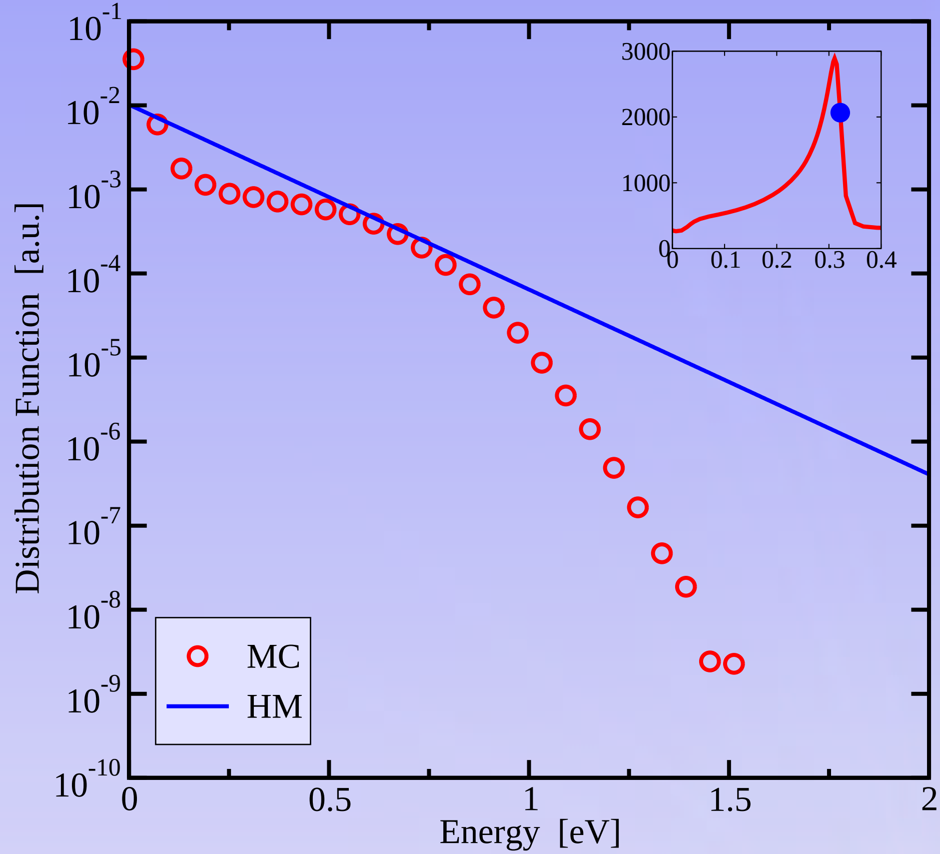

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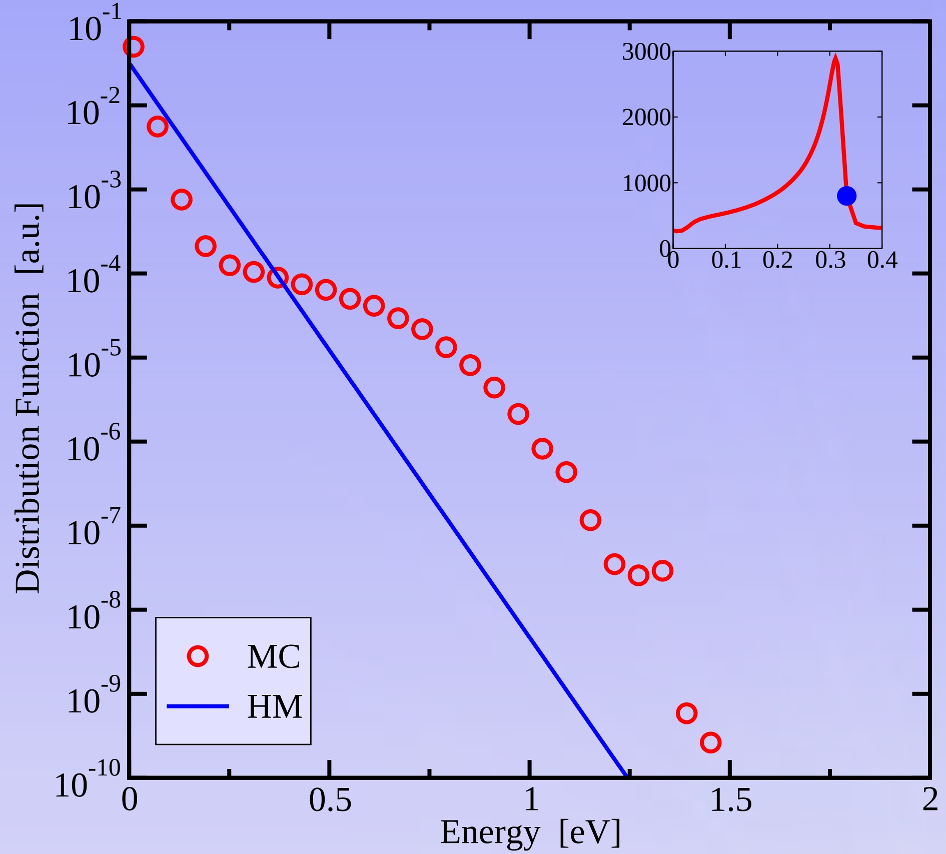

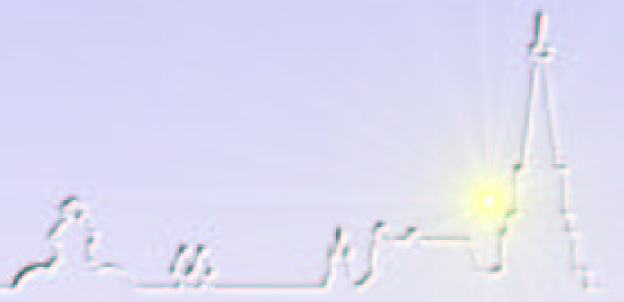

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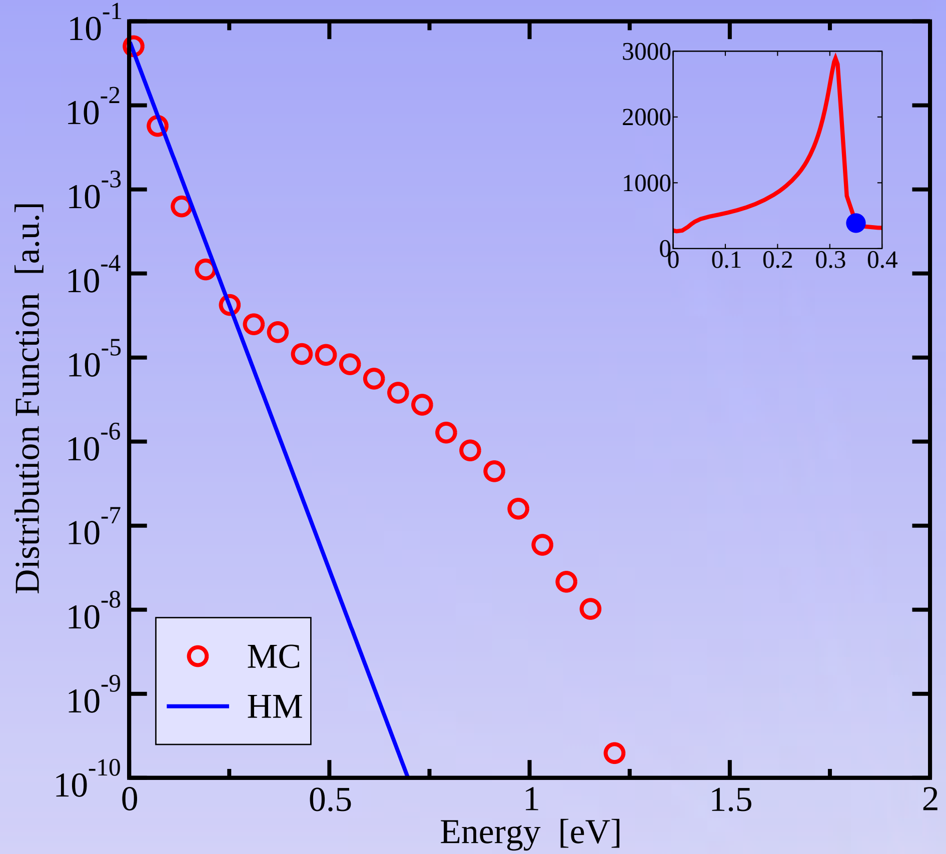

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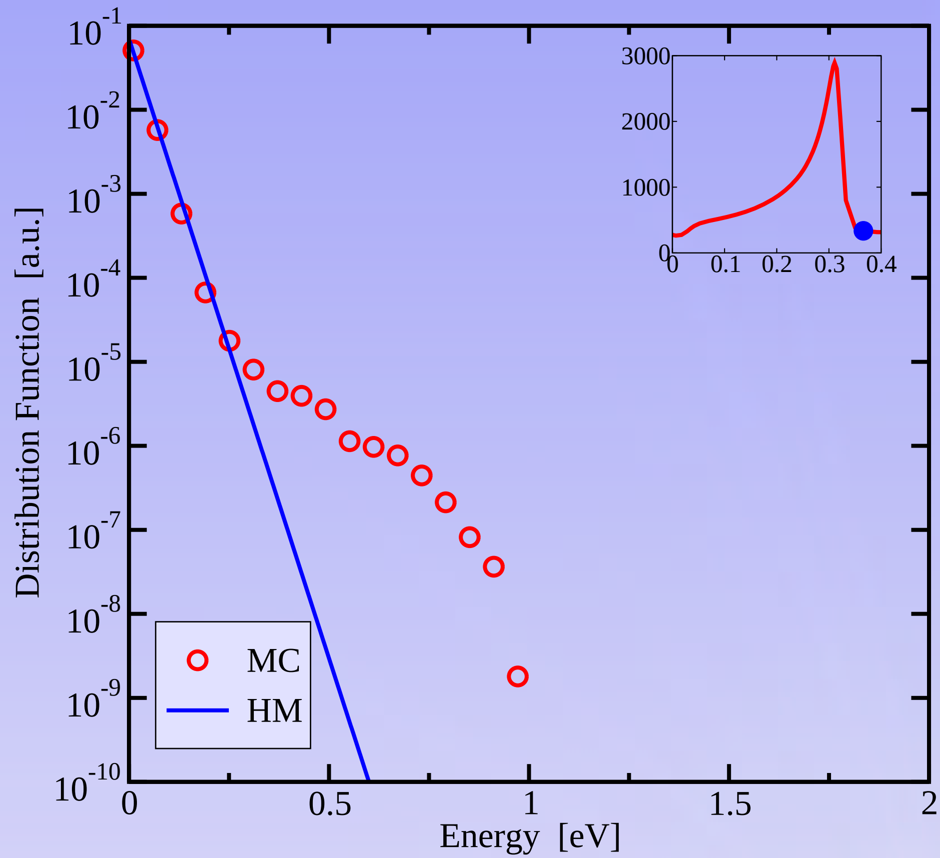

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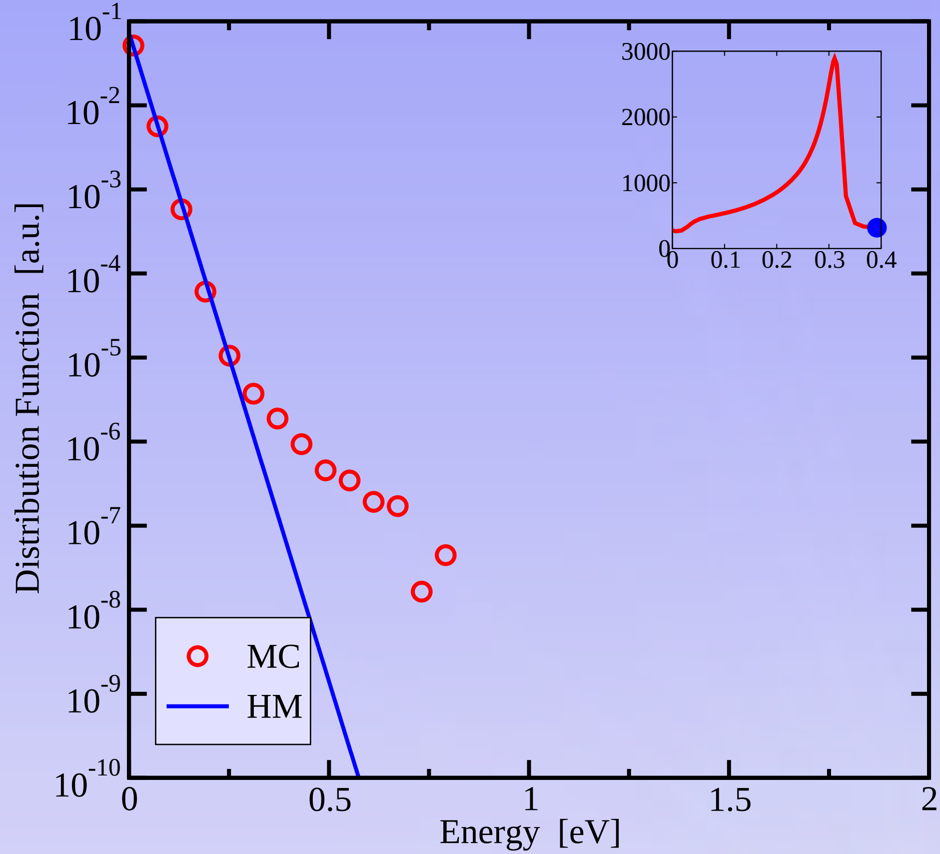

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  Deviation from Maxwellian

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- Distribution function model

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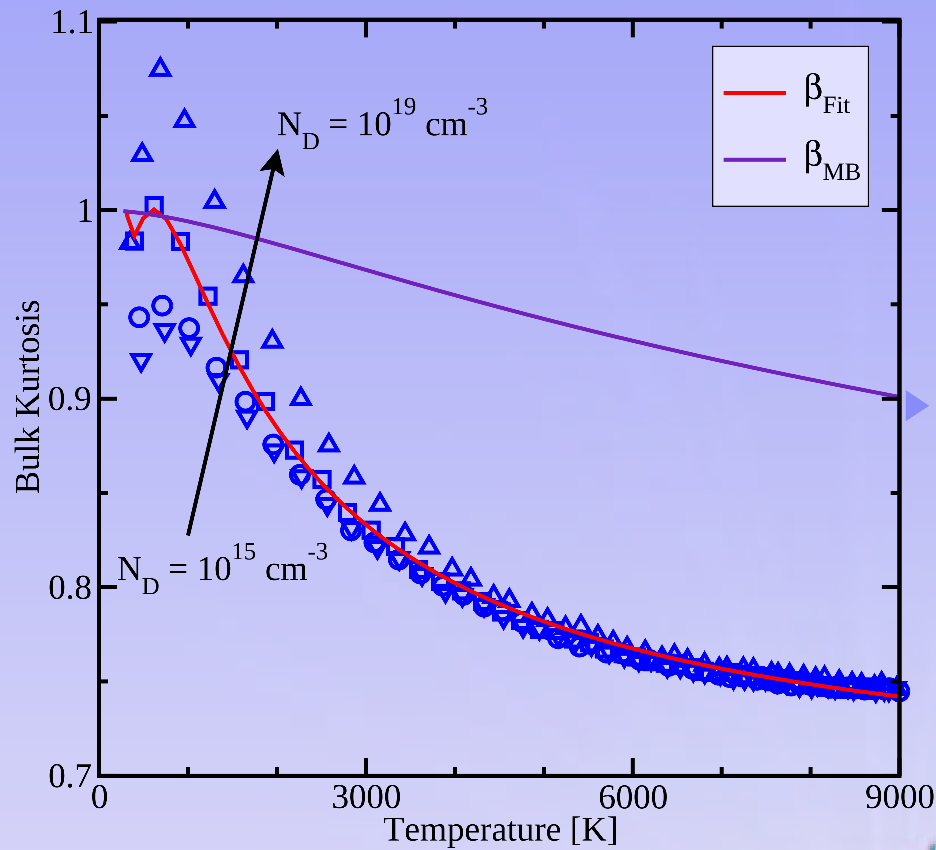

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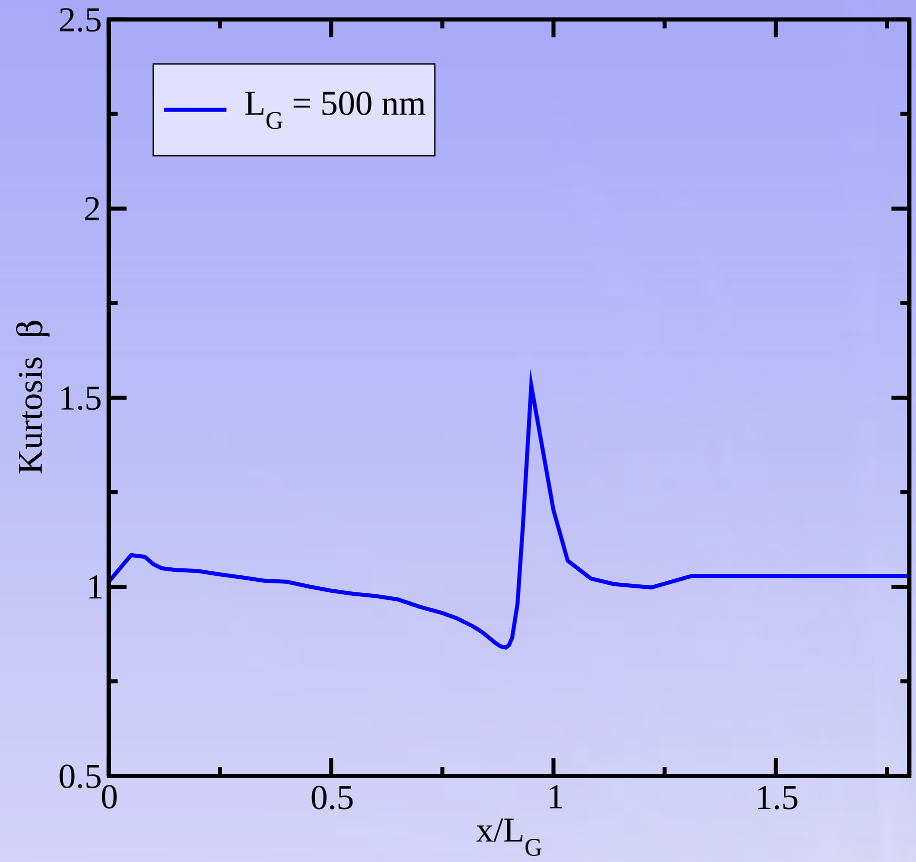

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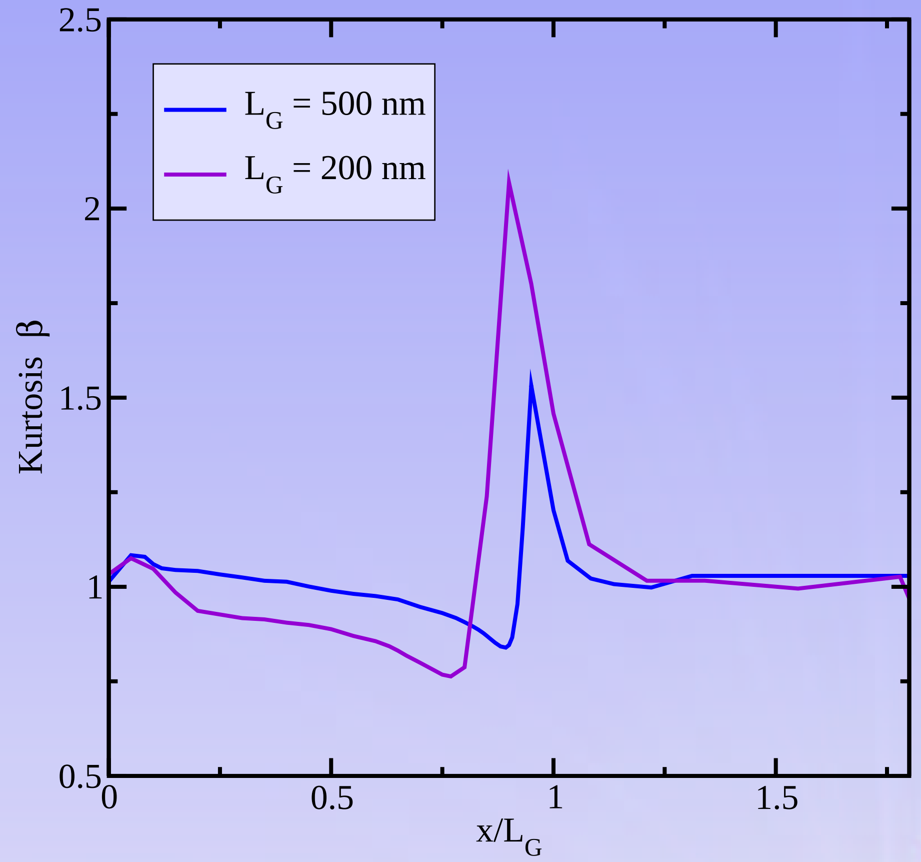

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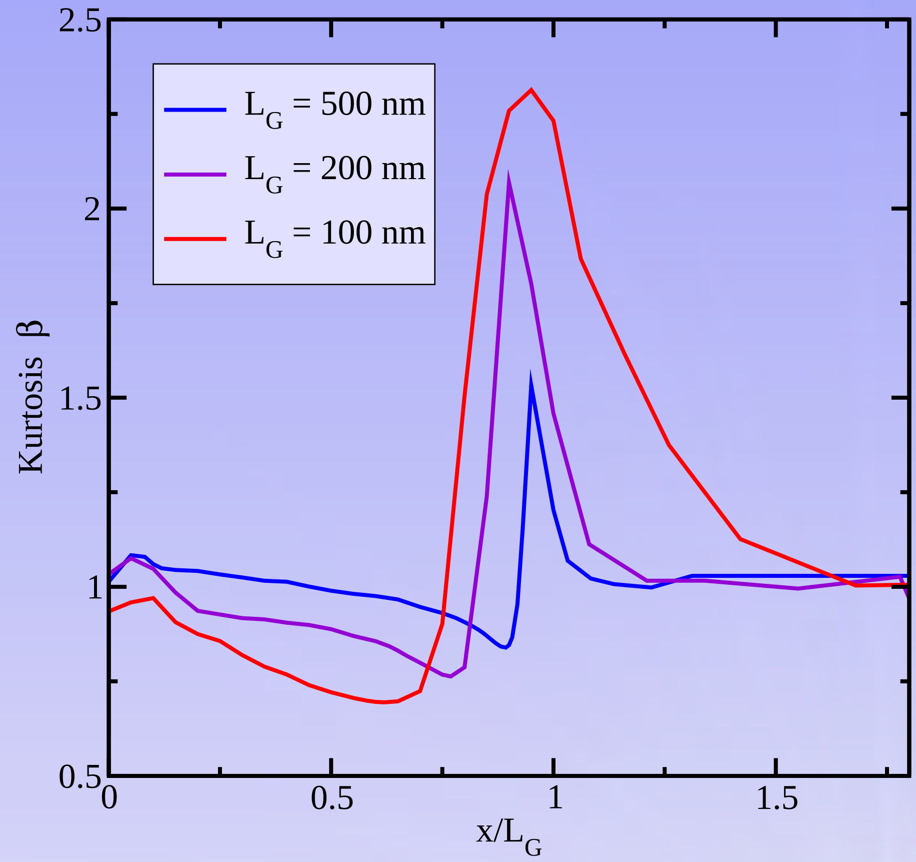

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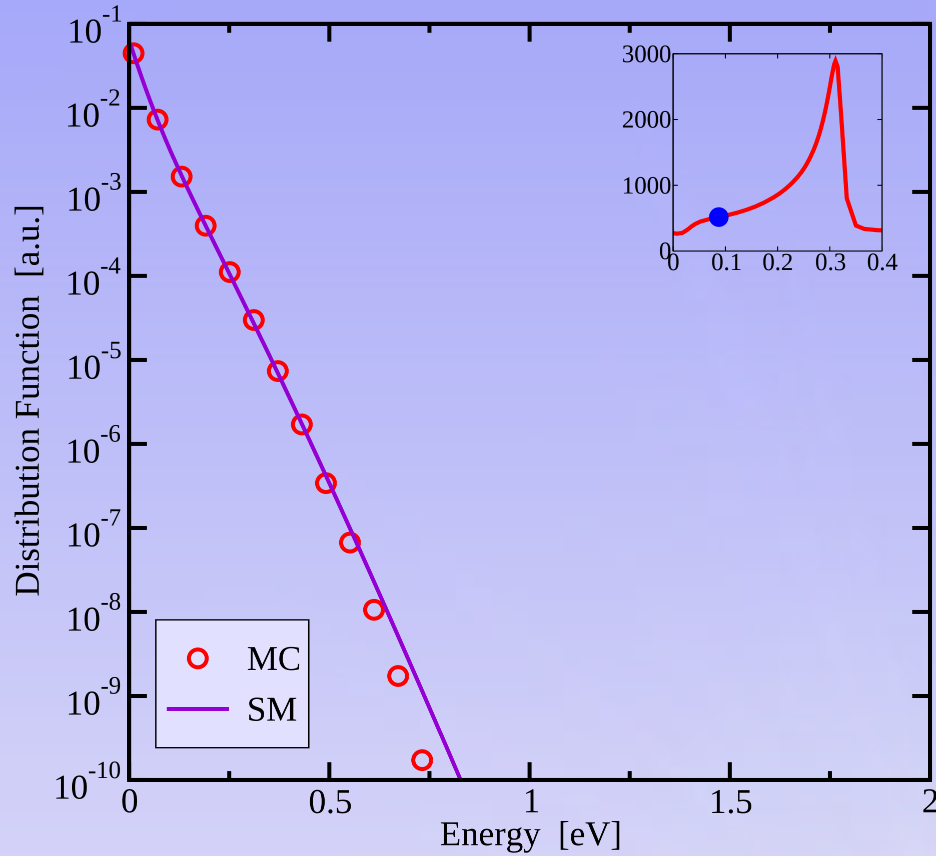

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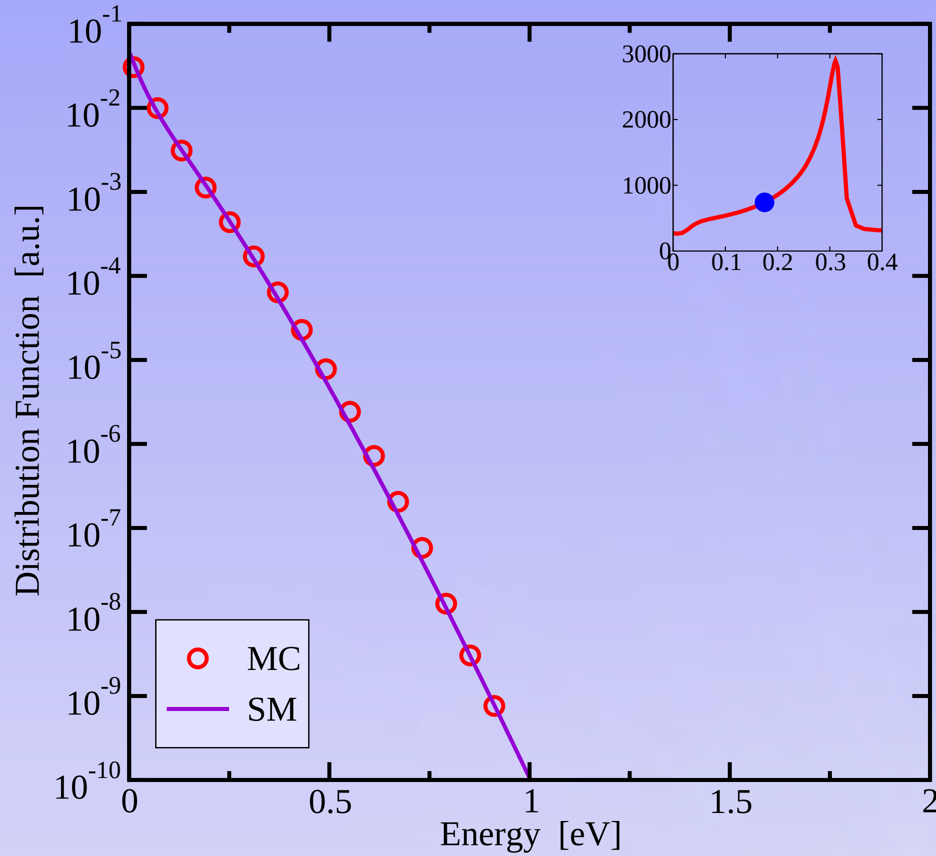

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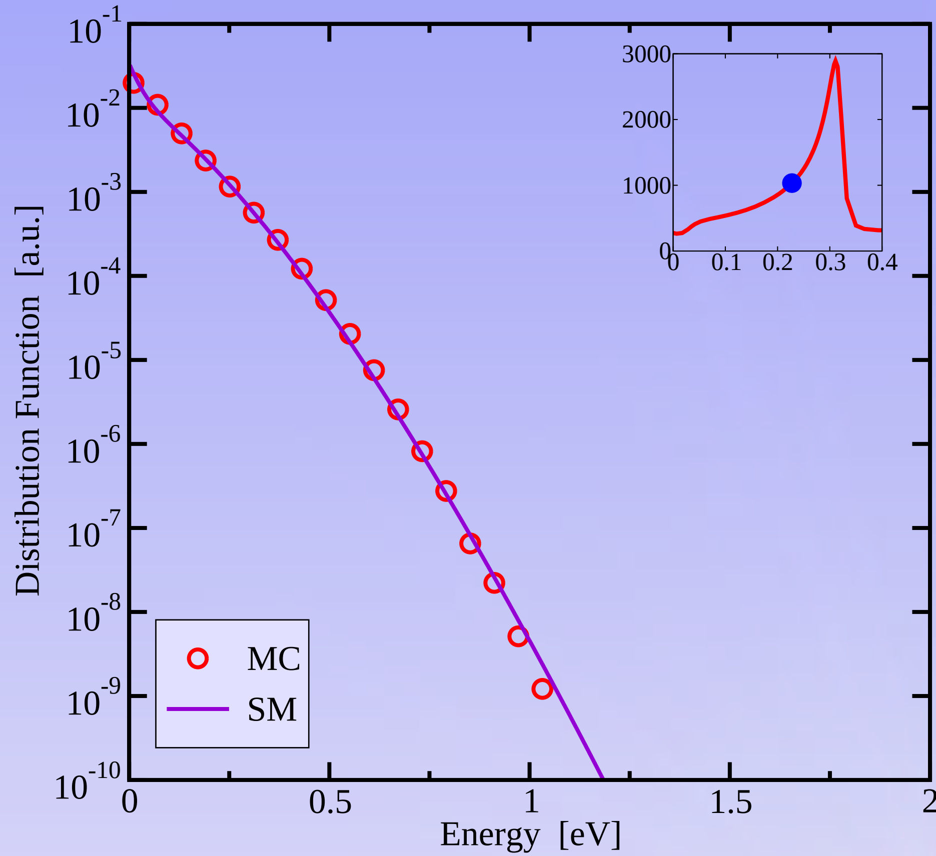

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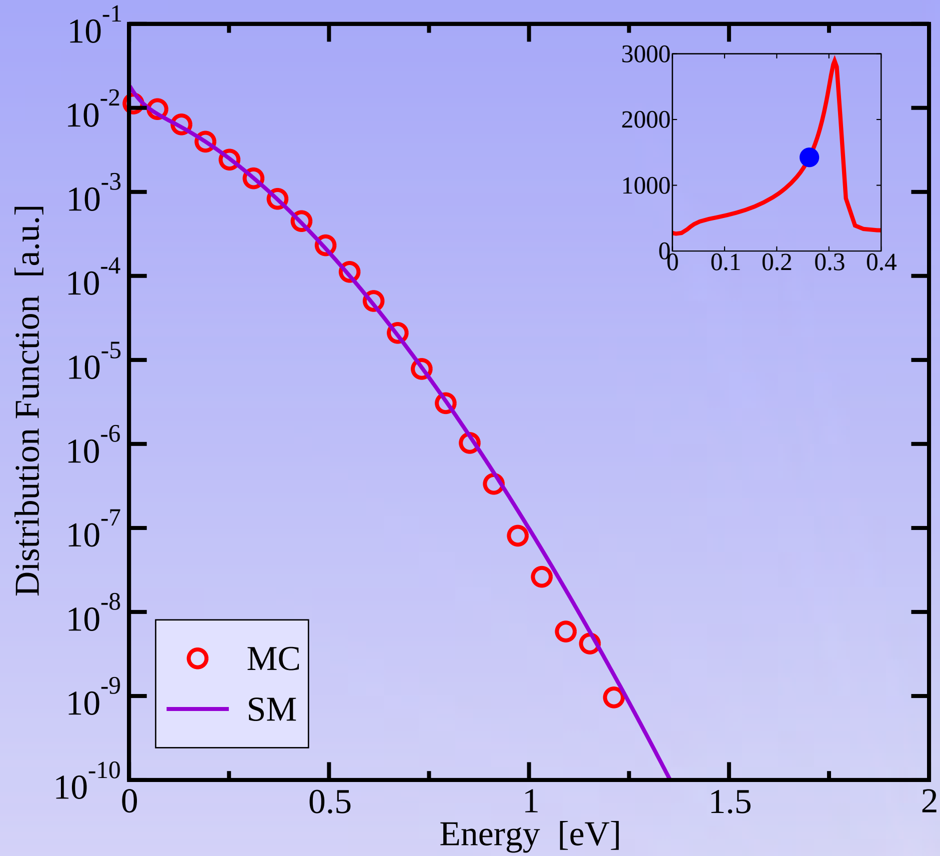

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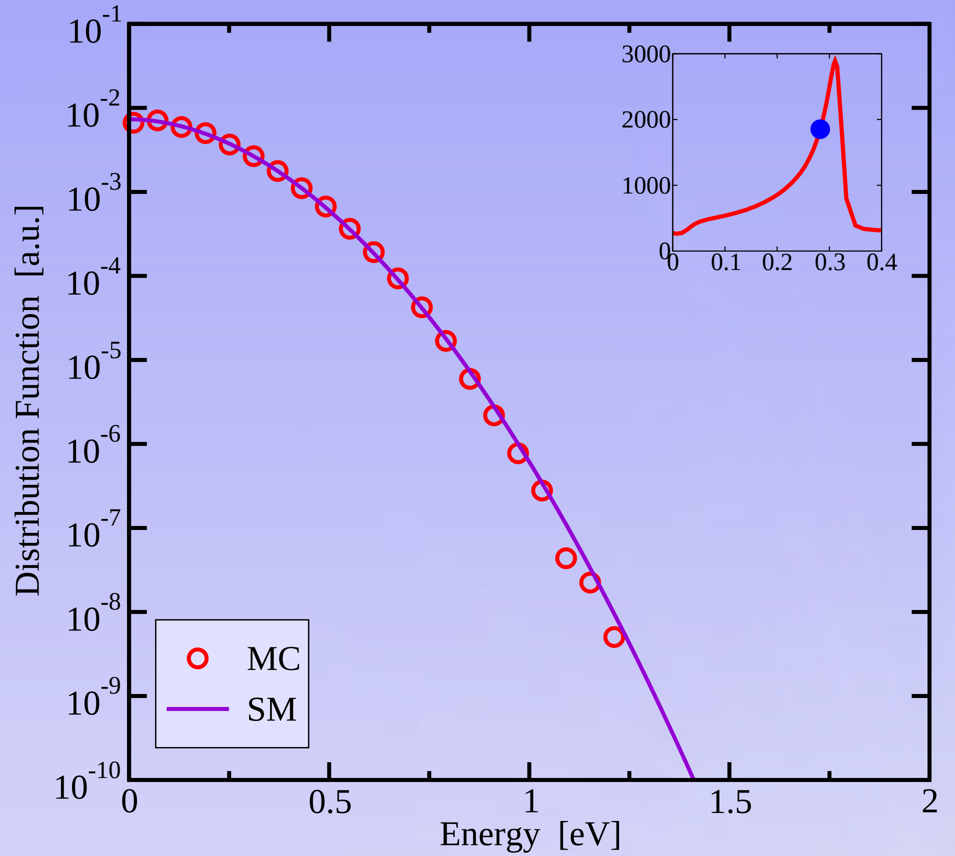

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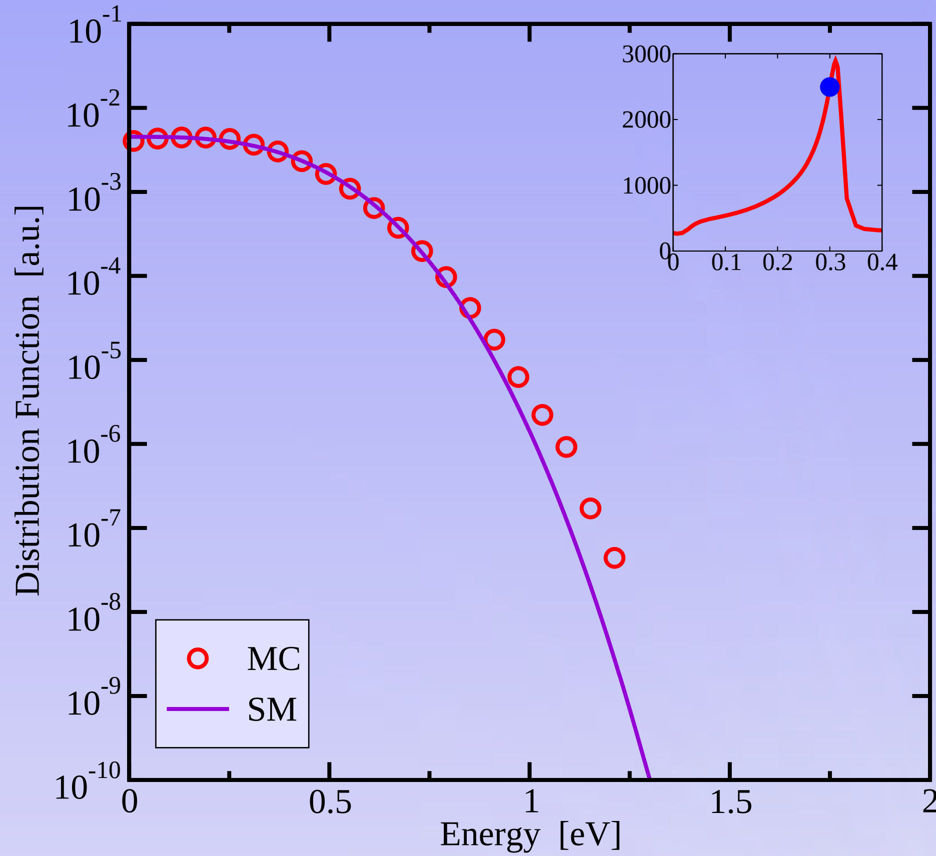

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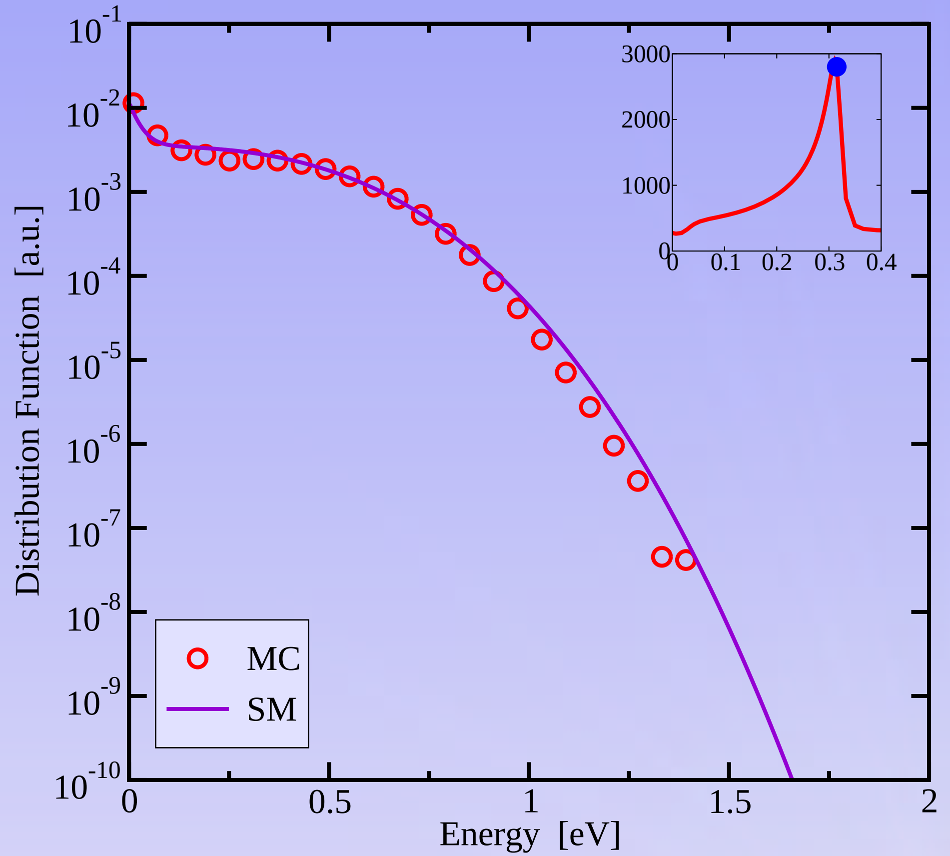

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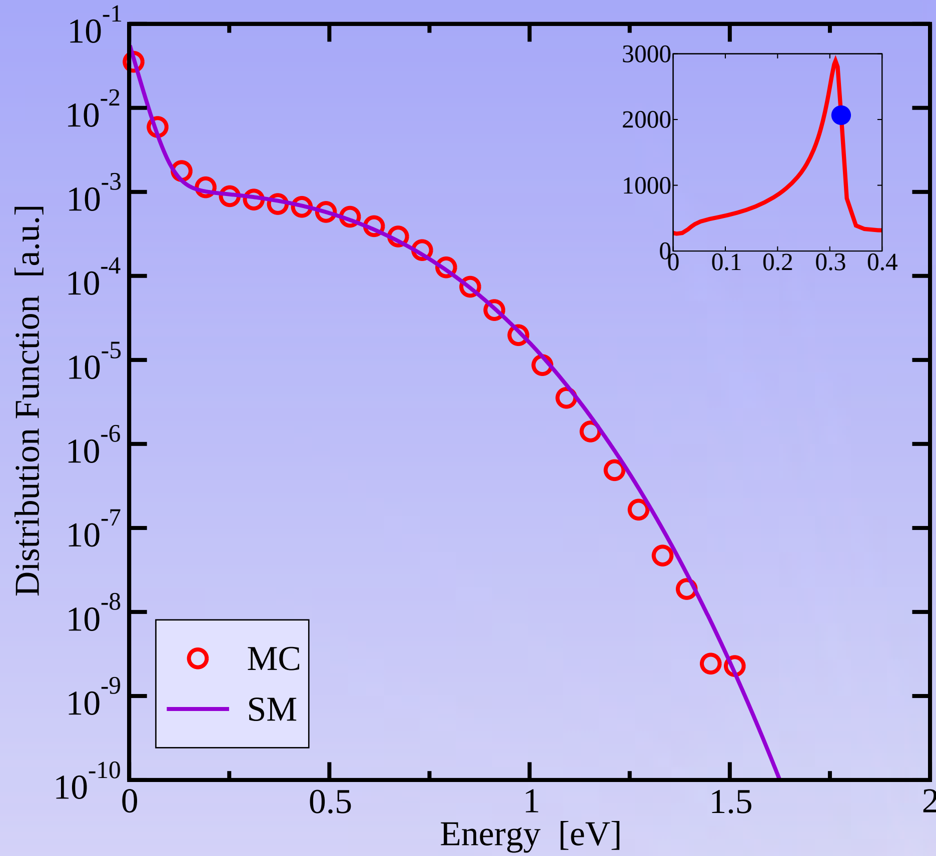

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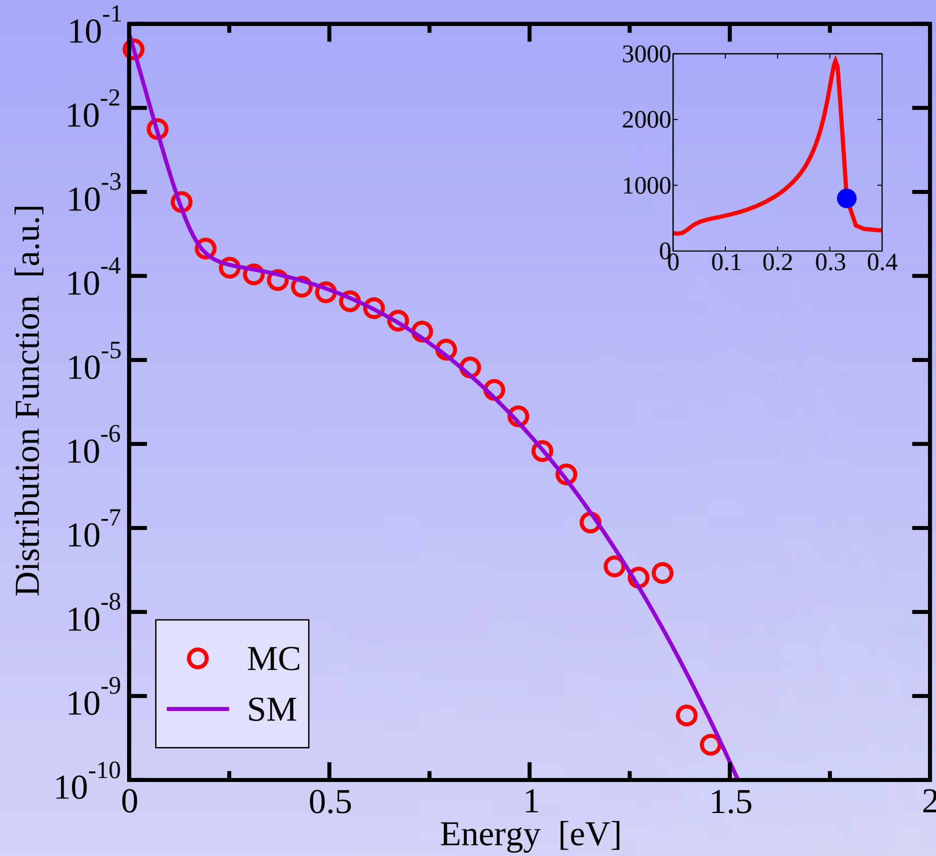

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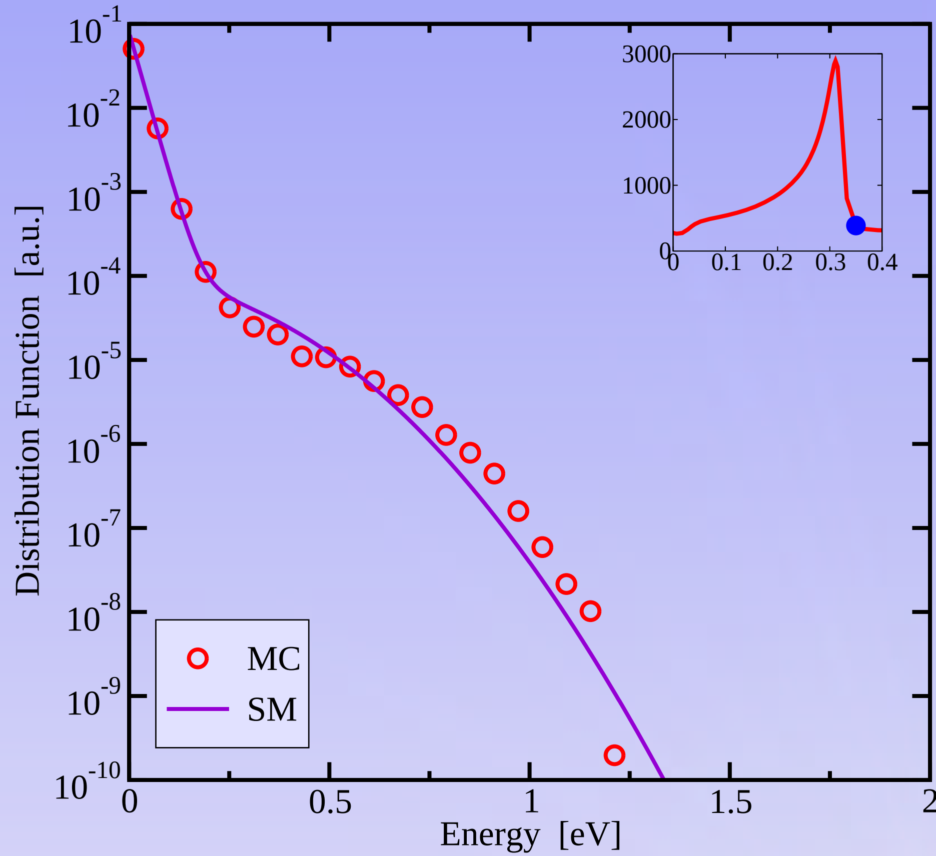


Anti-Symmetric Part

- Diffusion scaling of BTE, scaling parameter κ
- Diffusion limit of BTE ($\kappa \ll 1$), neglect terms $O(\kappa^2)$
- Displacing the symmetric part

$$f(\mathbf{k}) = f_{\mathrm{S}}(\mathbf{k} - \kappa\,\mathbf{k}_{\mathrm{c}}) \approx f_{\mathrm{S}}(\mathbf{k}) - \frac{\partial f(\mathbf{k})}{\partial \kappa} \cdot \kappa\,\mathbf{k}_{\mathrm{c}}, \qquad \mathbf{k}_{\mathrm{c}} = \sum_{i=0}^{2} \mathbf{k}_i \mathcal{E}^i$$

- Anti-Symmetric part must reproduce $\langle \mathbf{u}\mathcal{E}^i \rangle$

$$f_{\mathrm{A}}(\mathbf{k}) = f_{\mathcal{E}}(\mathcal{E}) \sum_{i=0}^{2} d_i(\mathcal{E})\,\langle \mathbf{u}\mathcal{E}^i \rangle \cdot \mathbf{k}$$

- Coefficients d_i depend only on the even moments $\langle \mathcal{E}^i \rangle$

Scattering Integral

- Standard scattering rates (Fermi's Golden Rule)

  Phonon scattering (acoustic and intravalley)

  Impurity scattering (Brooks-Herring)

- Mobilities

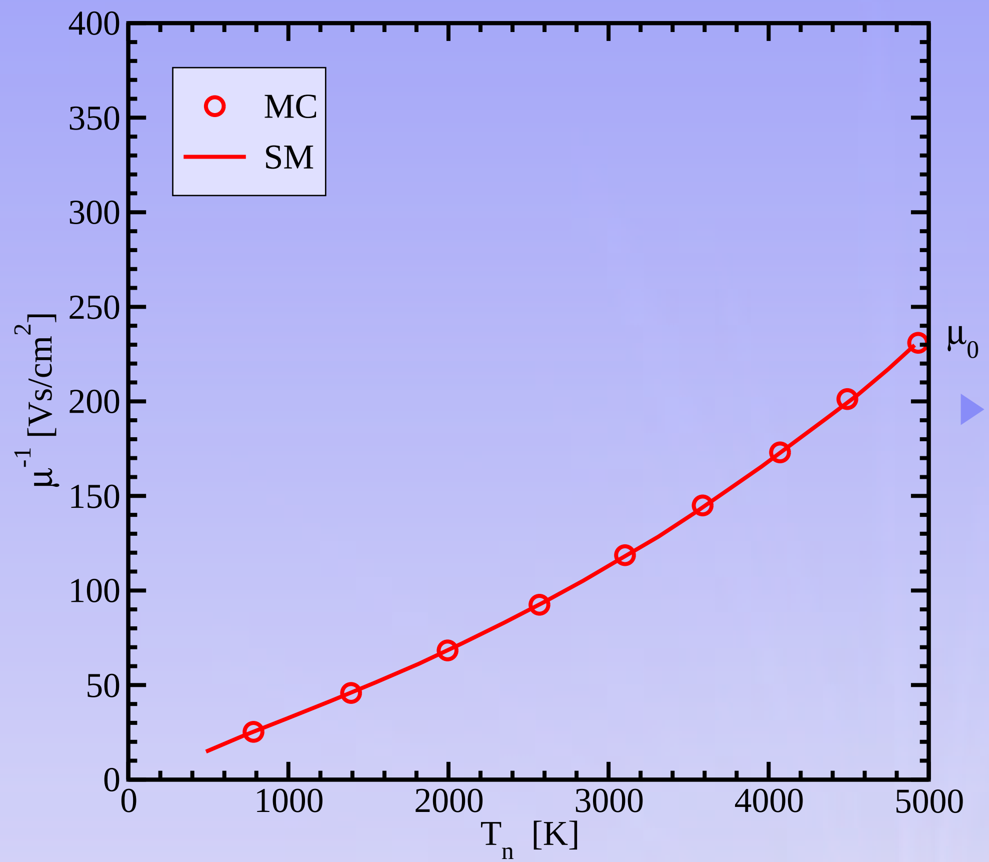
$$\frac{1}{n}\int \mathbf{p}\mathcal{E}^i\, Q[f]\ \mathrm{d}^3\mathbf{k} = -\left\langle \frac{\mathbf{p}\mathcal{E}^i}{\tau_p(\mathcal{E})} \right\rangle = -\mathrm{q}\,\frac{\langle \mathbf{u}\mathcal{E}^i \rangle}{\mu_i}$$

- Relaxation times

$$\frac{1}{n}\int \mathcal{E}^i\, Q[f]\ \mathrm{d}^3\mathbf{k} = -\left\langle \frac{\mathcal{E}^i}{\tau_{\mathcal{E}^i}(\mathcal{E})} \right\rangle = -\frac{\langle \mathcal{E}^i \rangle - \langle \mathcal{E}^i \rangle_{\mathrm{eq}}}{\tau_i}$$

Results

- Bulk
- Mobilities



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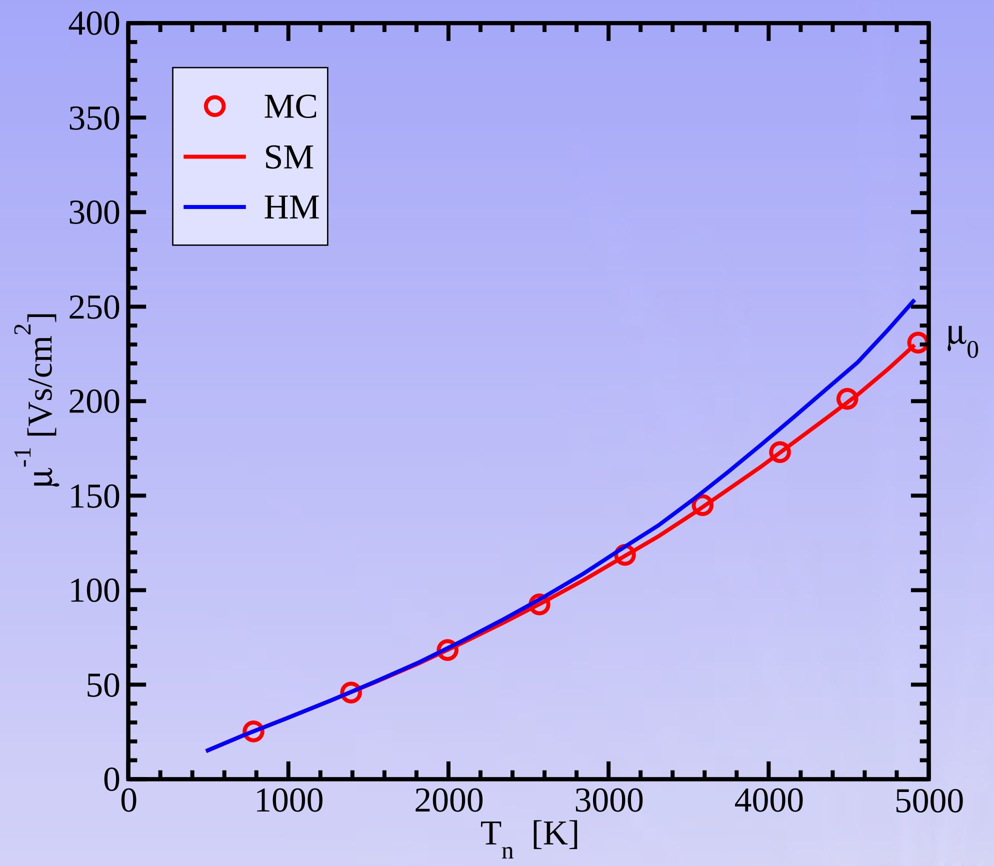

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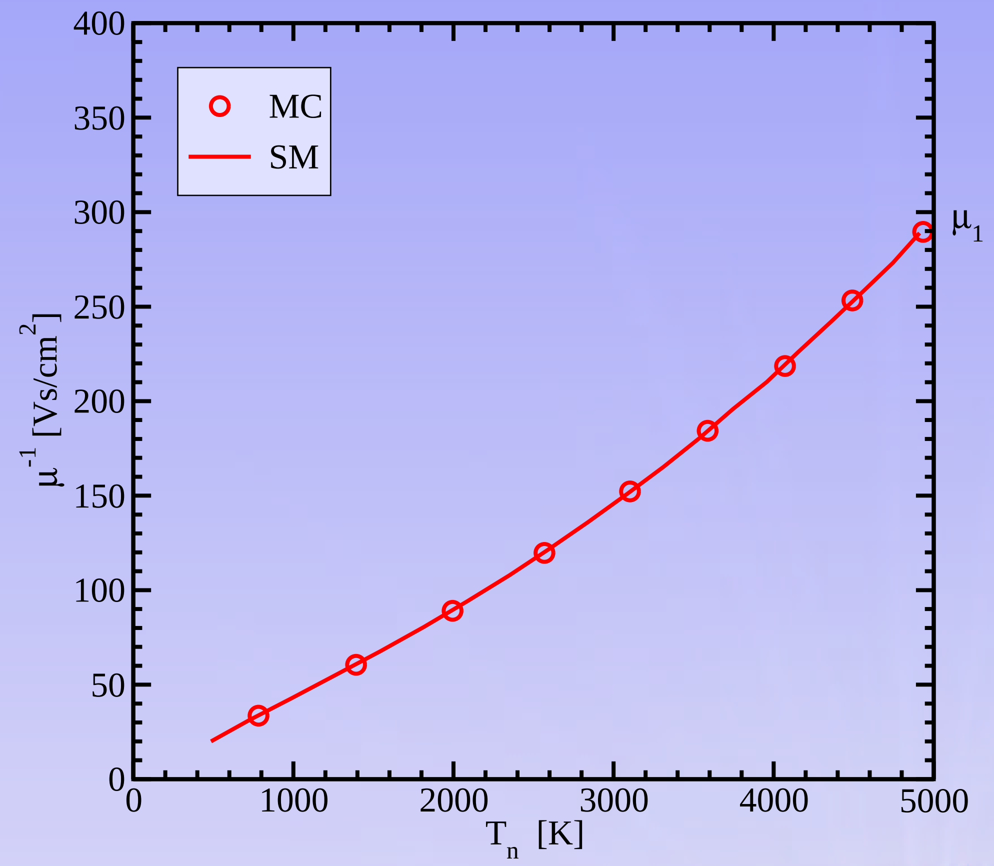

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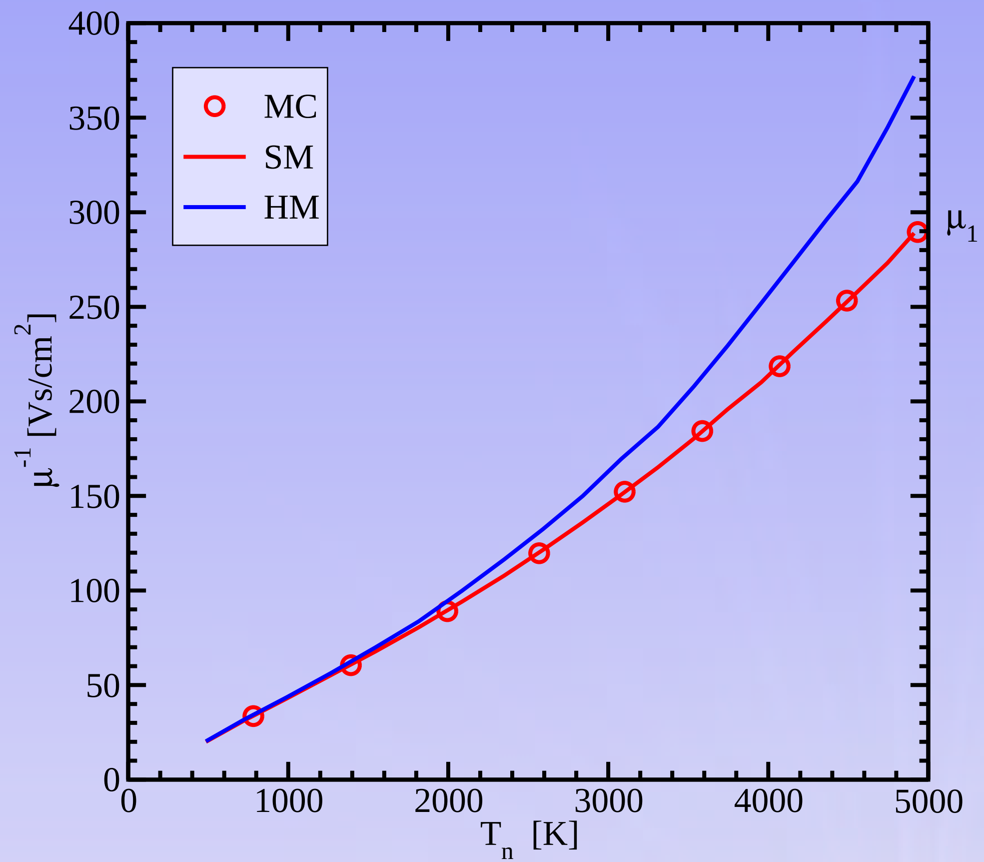

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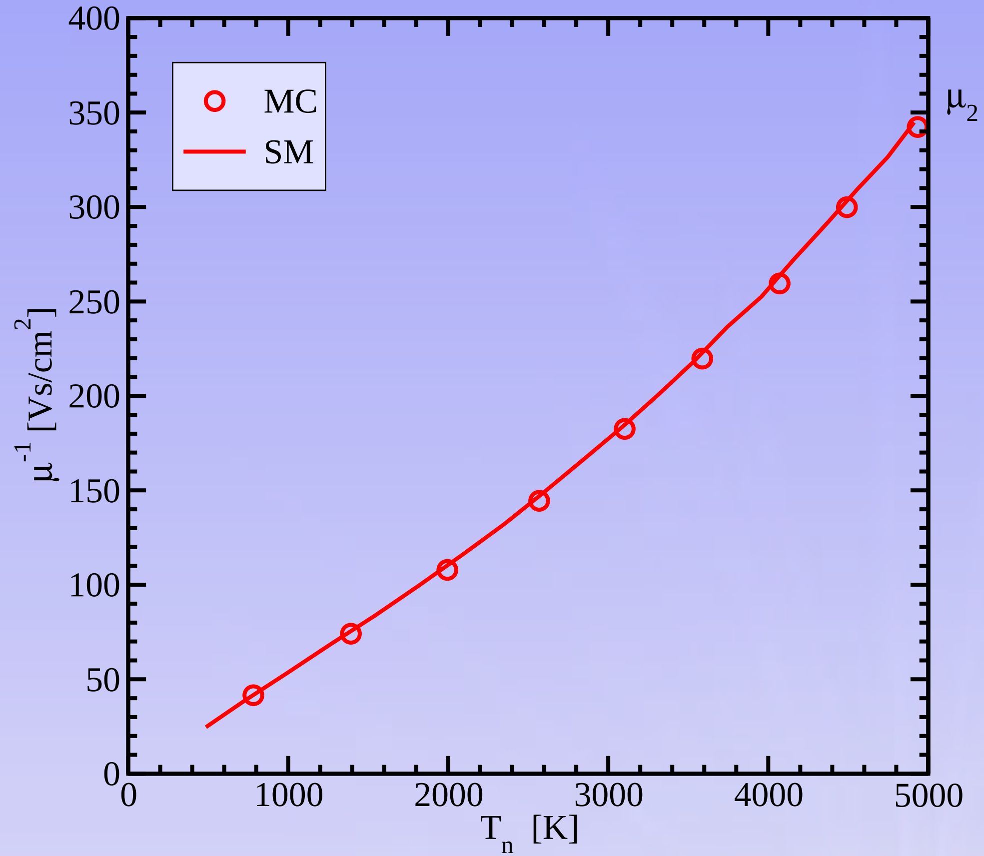

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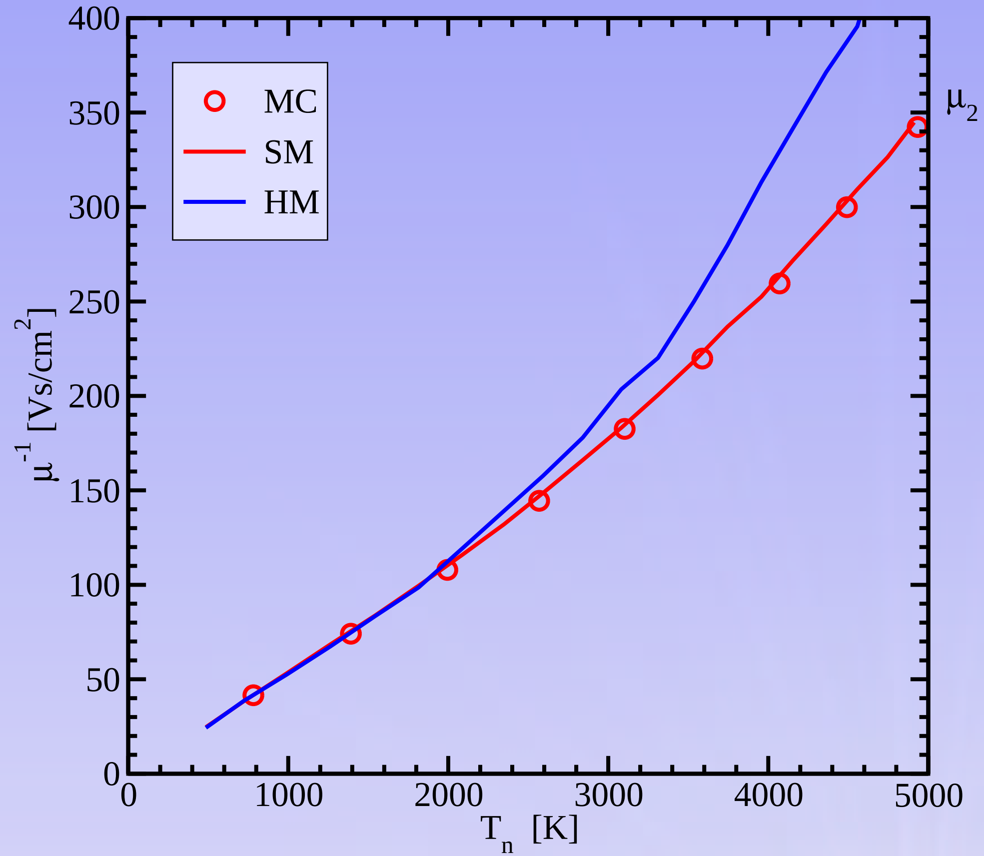
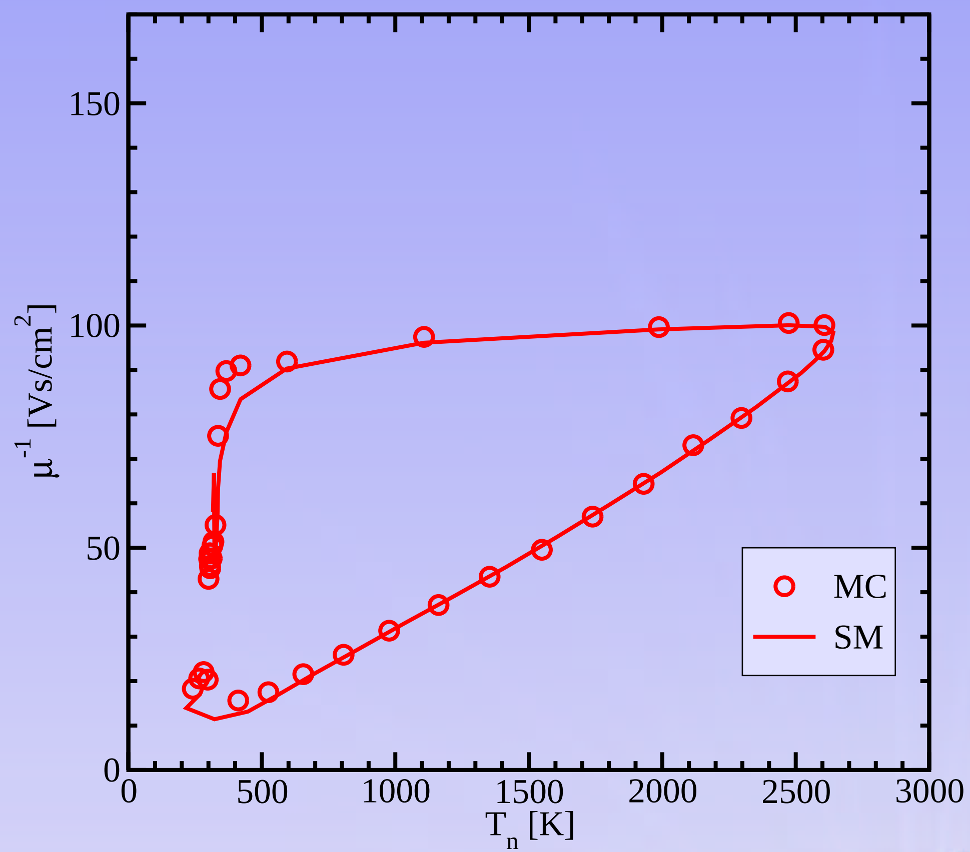


Results

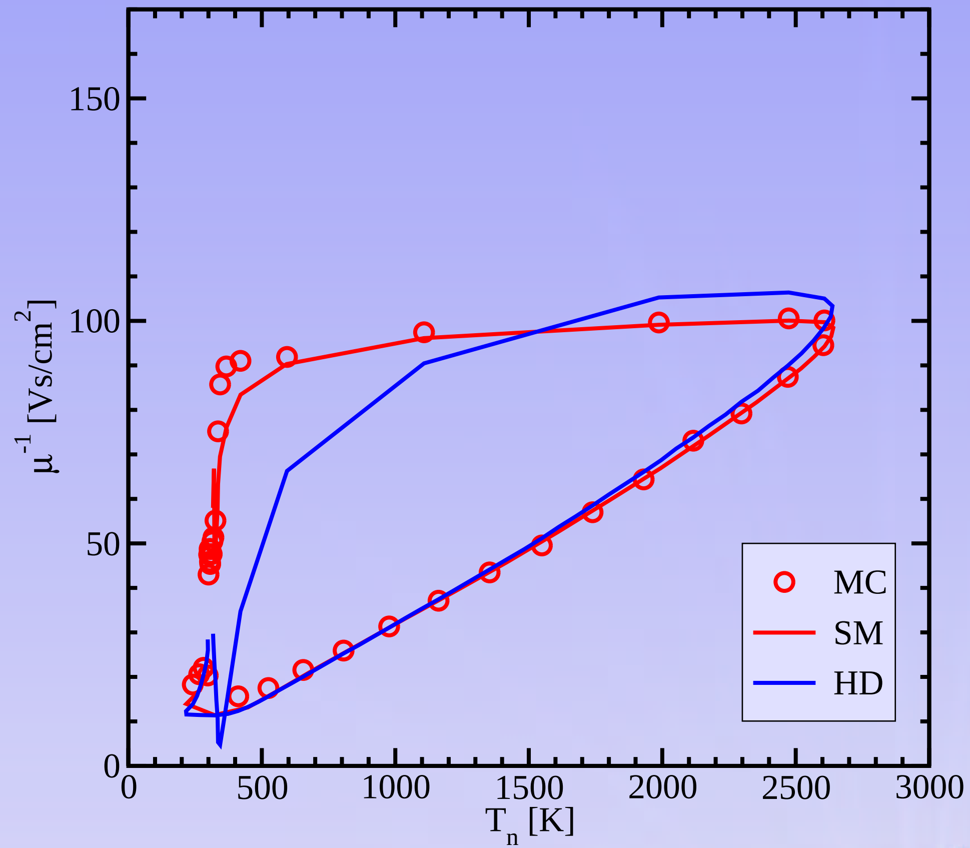
- n^+-n-n^+ with $L_{\mathrm{C}} = 100$ nm
- Mobilities



Results

- n^+-n-n^+ with $L_C = 100$ nm
- Mobilities

  HM inaccurate in drain region



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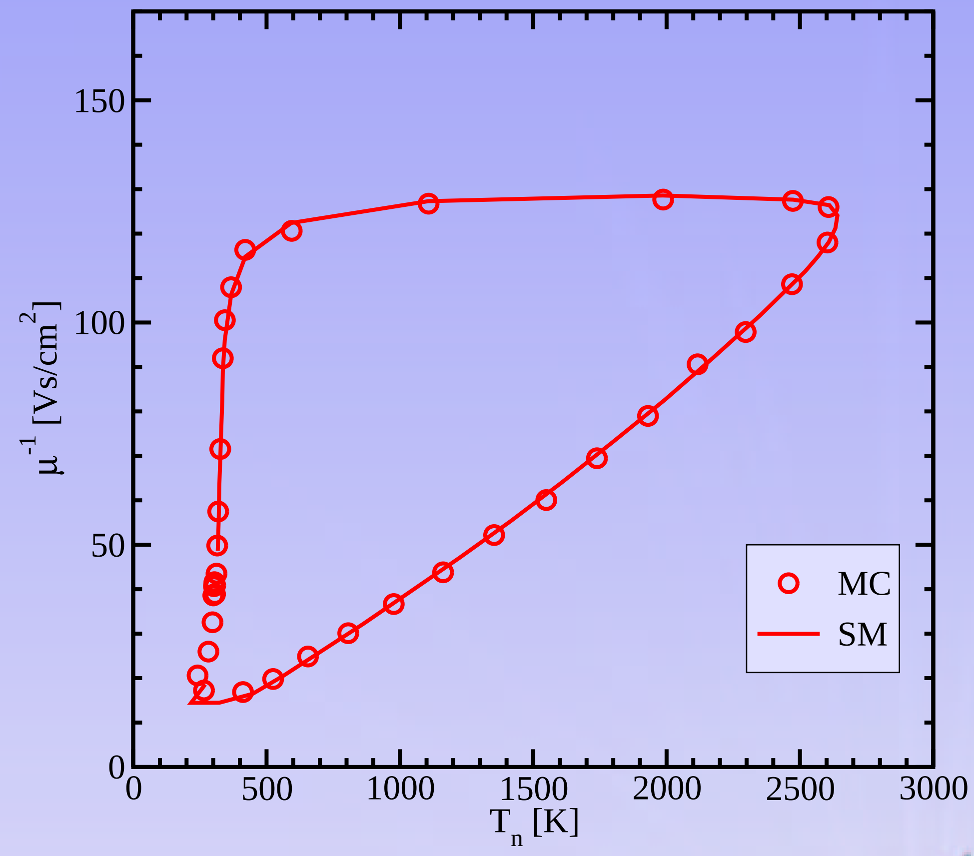
- Mobilities

  HM inaccurate in drain region

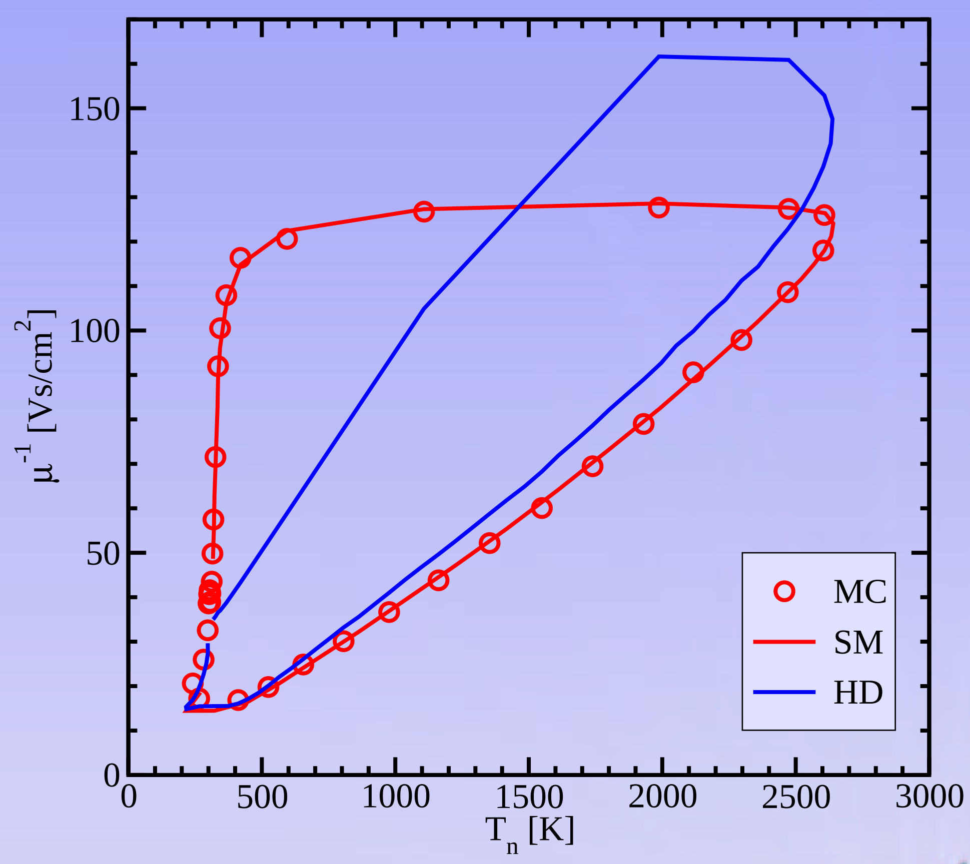


Results

- n^+-n-n^+ with $L_\mathrm{C} = 100\ \mathrm{nm}$
- Mobilities

  HM inaccurate in drain region

  particularly for μ_1



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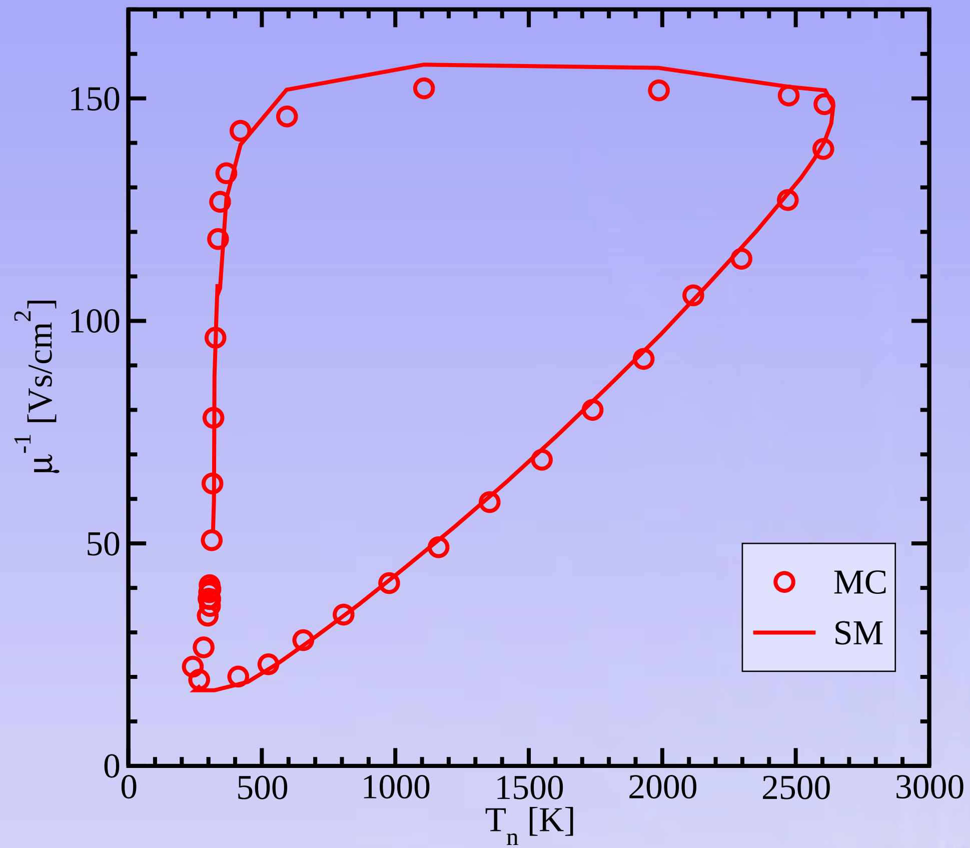

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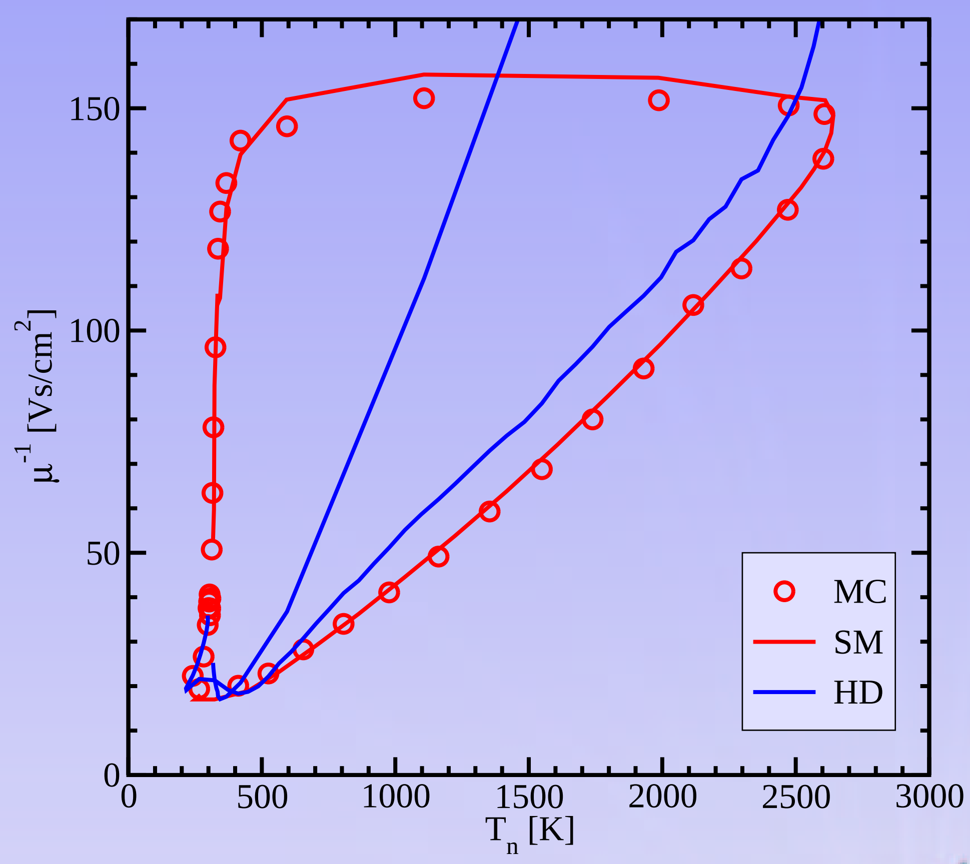

Results

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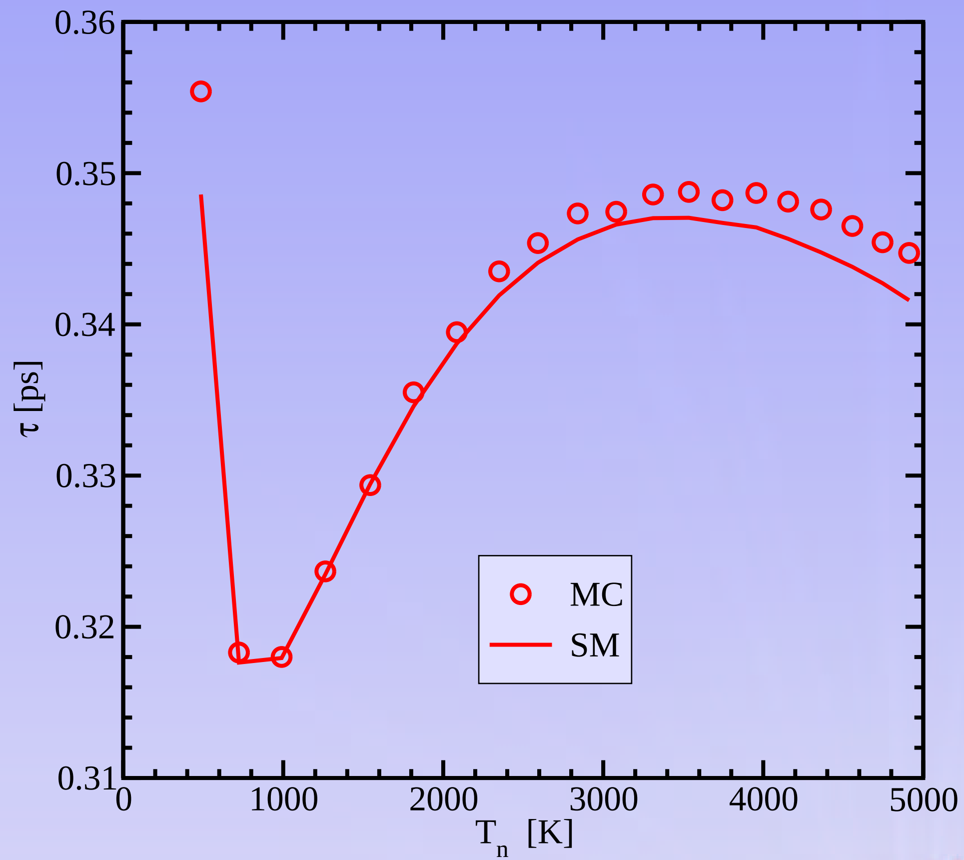
- Mobilities

  HM inaccurate in drain region

  particularly for μ_1
- Relaxation Times



Results

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- Mobilities

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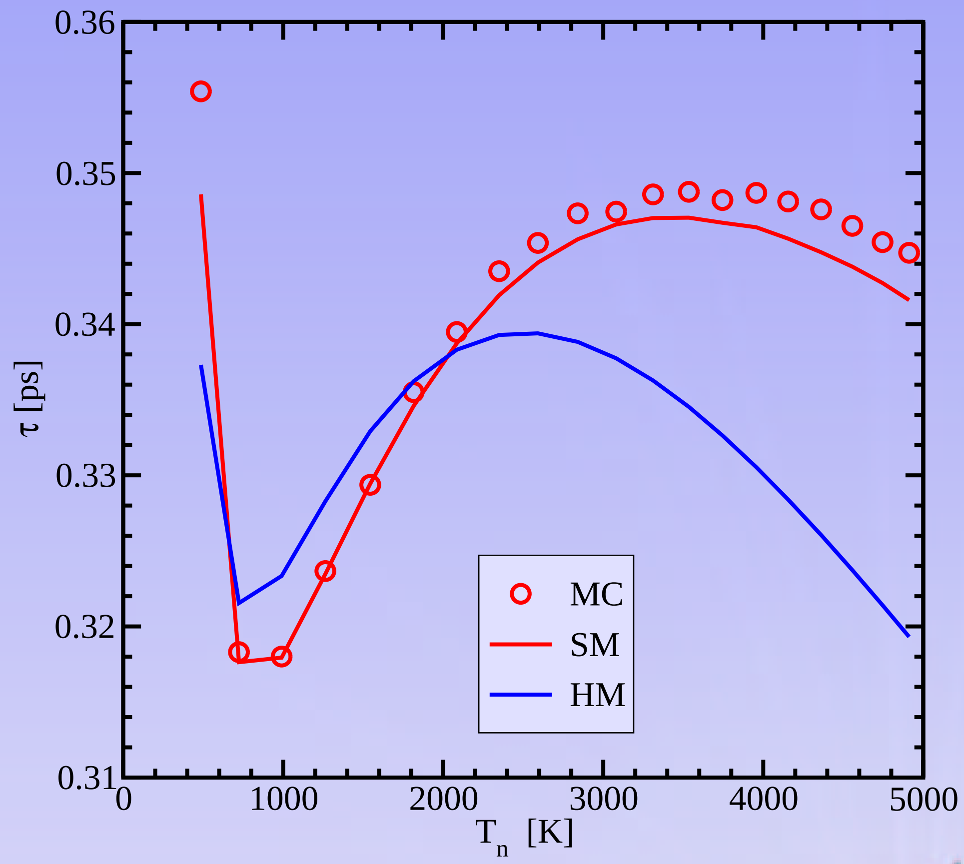
- Relaxation Times

  Single valued function



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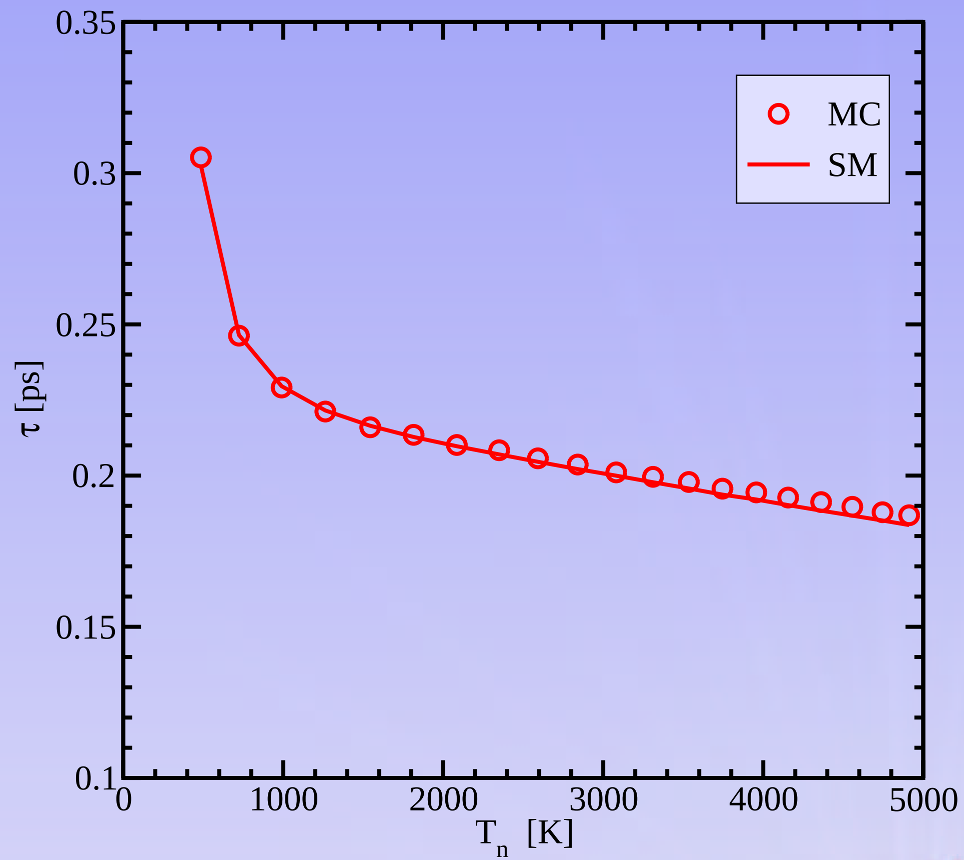

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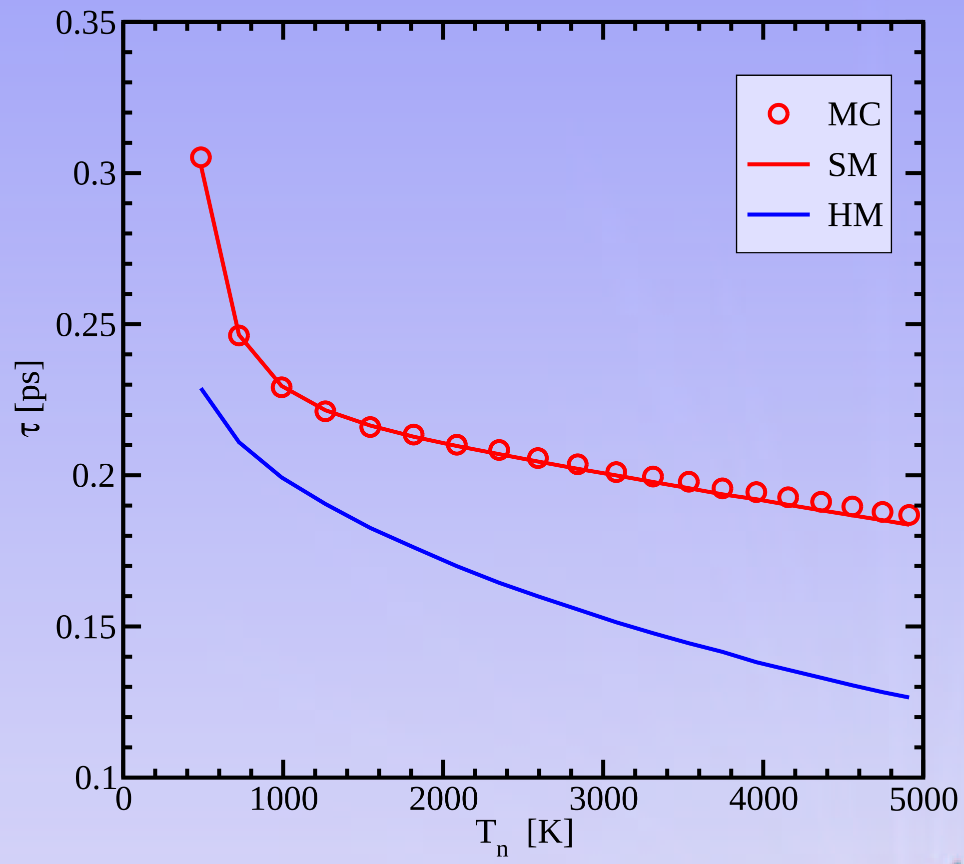

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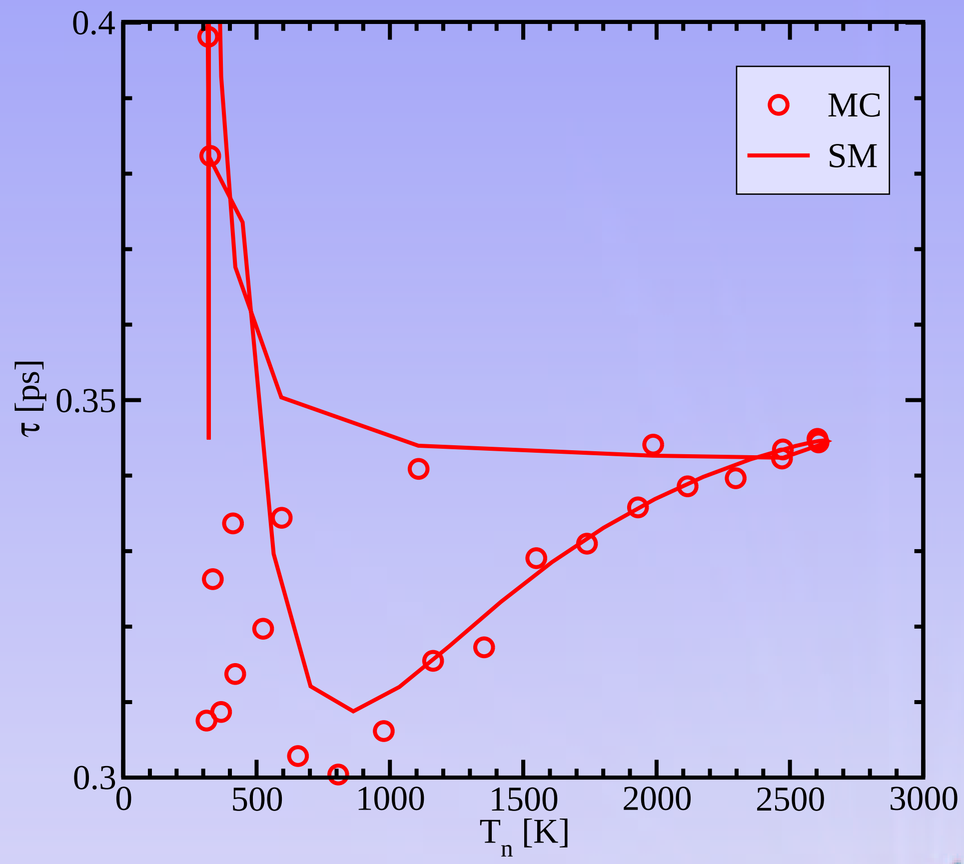

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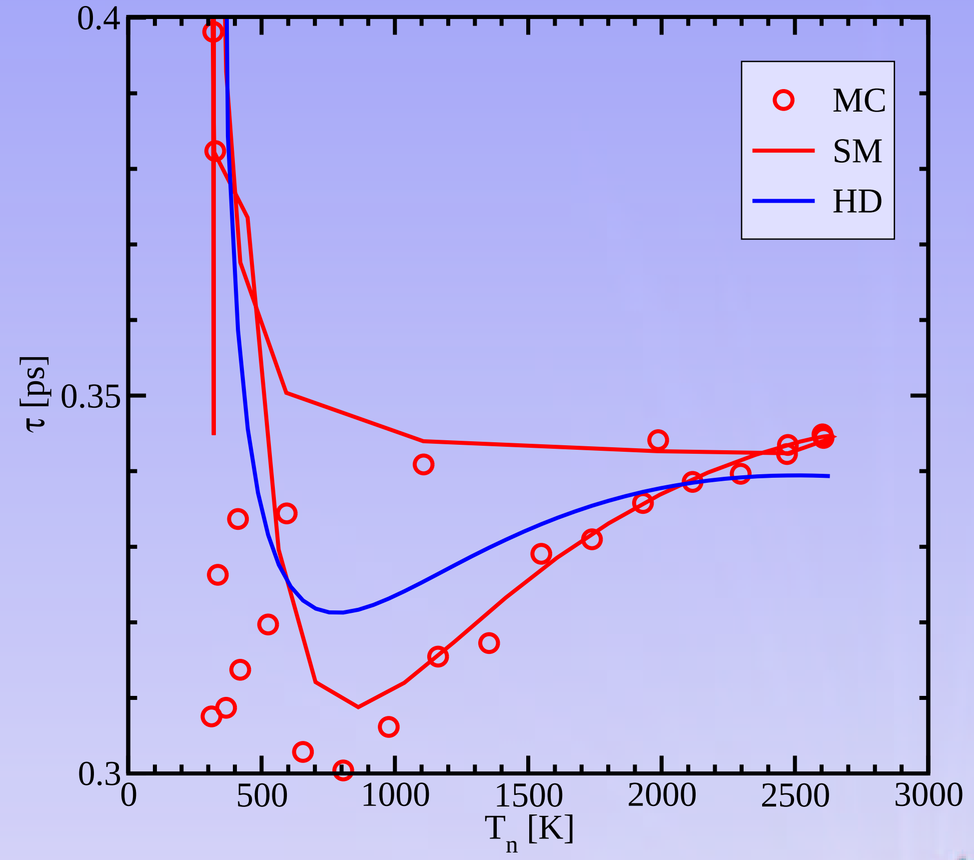

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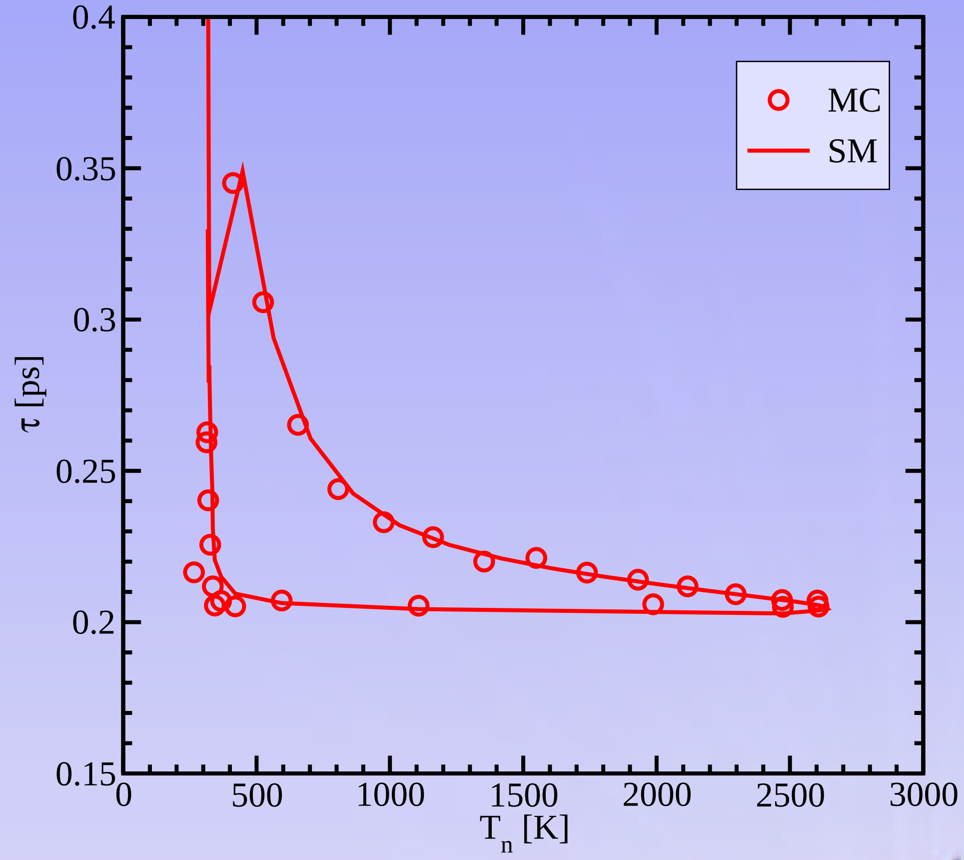

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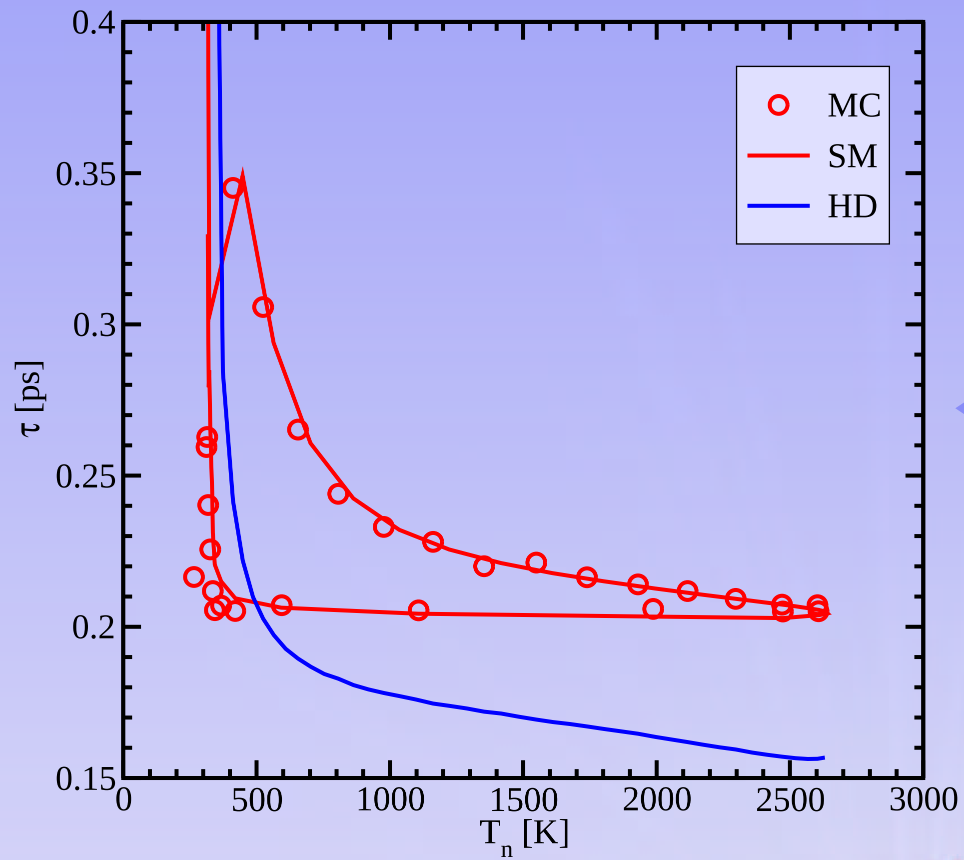

Conclusions

- Problems of energy-transport model
  - Scattering integral difficult to model
  - Closure assumes heated Maxwellian distribution
  - Only average energy known about distribution function
- Six moments model
  - Additional information about distribution function
  - Accurate description of distribution function
  - Transfer of microscopic models into macroscopic models
  - Accurate modeling of relaxation times and mobilities
  - Self-contained in contrast to energy-transport model