mpsd

Ab-initio Quantum Electrodynamics: Beyond the Model Paradigm

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[4] Center for Computational Quantum Physics, Flatiron Institute, New York, USA

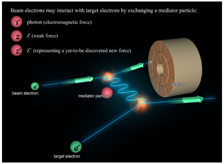
MOLECULAR POLARITONICS 2019

Theoretical and Numerical Approaches

Miraflores de la Sierra, Madrid, July 8, 2019

Introduction and motivation

Light and matter (quantum electrodynamics)



project.slac.stanford.edu/e158/experiment.html

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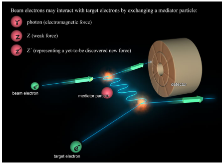

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- $\hat{H}_{\text{int}} = \frac{1}{c}\int \mathrm{d}^3 r \, \hat{J}_\mu(\mathbf{r}) \hat{A}^\mu(\mathbf{r})$

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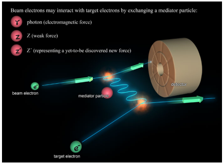

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- $\hat{H}_{\text{int}} = \frac{1}{c} \int \mathrm{d}^3 r \hat{J}_\mu(\mathbf{r}) \hat{A}^\mu(\mathbf{r})$
- $\hat{J}_\mu(\mathbf{r})$ charge current

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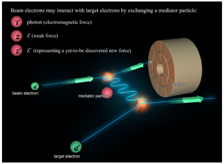

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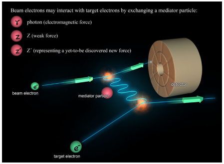

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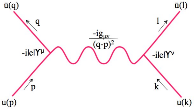
Matter (q-mechanics)



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Introduction and motivation

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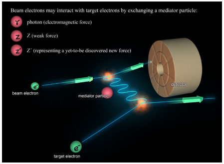

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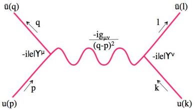

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- $\hat{H}_{\text{int}} \rightarrow \sum_{i>j}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$

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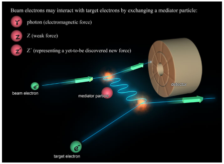

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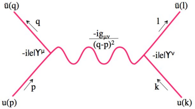

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- $\hat{H}_{\text{int}} \to \sum_{i>j}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$
- Particles only

Introduction and motivation

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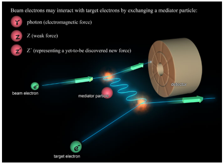

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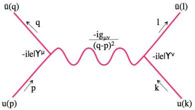

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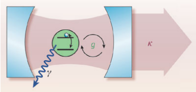
Light (q-optics)



Schoelkopf *et al.*, Nature **451**, 664 (2008)

Introduction and motivation

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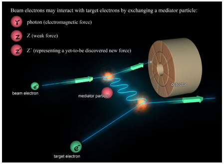

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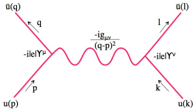

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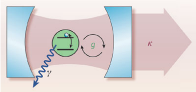

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- $\hat{H}_{int} \rightarrow \sum \boldsymbol{\lambda}_k(\hat{a}_k + \hat{a}^\dagger_k)\cdot\hat{\boldsymbol{R}}$

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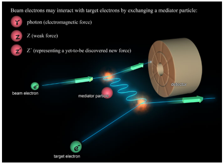

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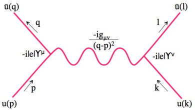

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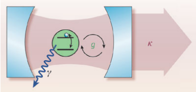
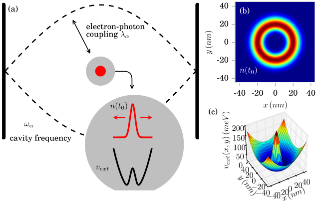


Schoelkopf *et al.*, Nature **451**, 664 (2008)

- $\hat{H}_{int} \rightarrow \sum \boldsymbol{\lambda}_k(\hat{a}_k + \hat{a}^\dagger_k)\cdot\hat{\boldsymbol{R}}$
- Few modes and levels

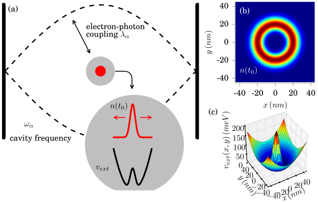
Limitations of models and standard approximations[1,2]



GaAs quantum ring in a cavity (weak coupling).

[1] C. Schäfer *et al.*, PRA **98**, 043801 (2018), [2] M. Sentef *et al.*, Science Adv. **4** (11), eaau6969 (2018)

Limitations of models and standard approximations[1,2]



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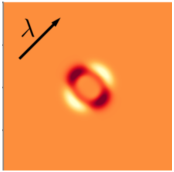

$n_\lambda - n_0$ (exact)

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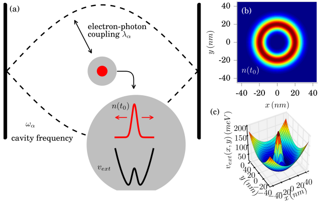

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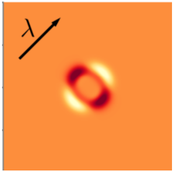

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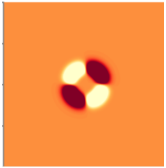

$n_\lambda - n_0$ (three levels)

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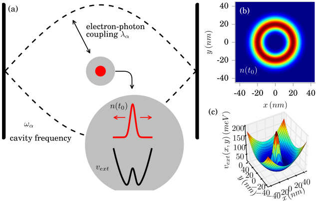

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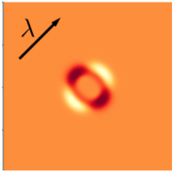

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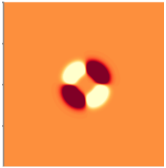

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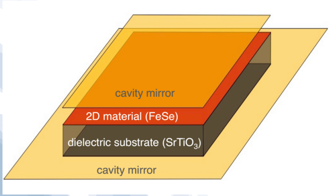

Superconductor in cavity (strong coupling)

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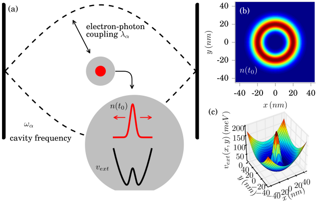

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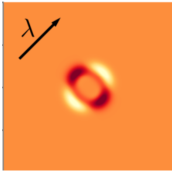

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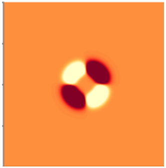

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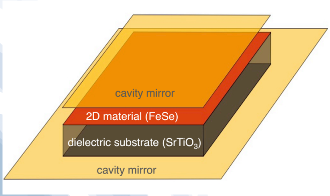

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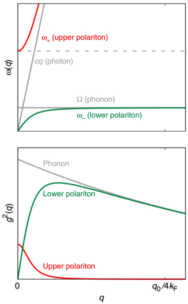

exact

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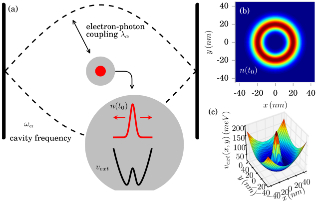
Limitations of models and standard approximations[1,2]



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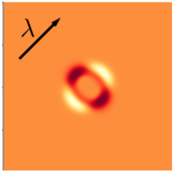

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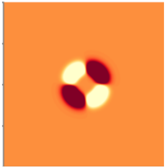

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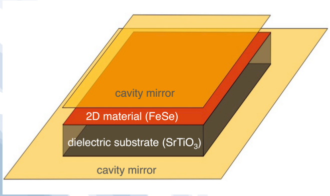

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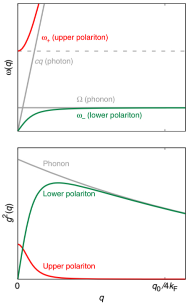

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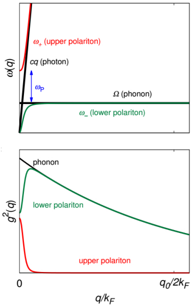
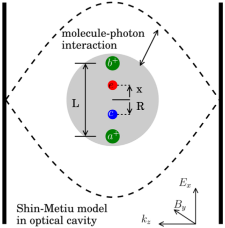


rotating wave approximation

[1] C. Schäfer *et al.*, PRA **98**, 043801 (2018), [2] M. Sentef *et al.*, Science Adv. **4** (11), eaau6969 (2018)

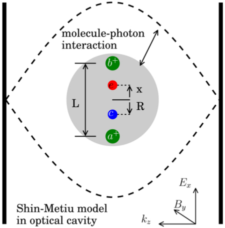
Limitations of models and standard approximations[3,4,5]



Molecule (strong coupling).

[3] J. Flick *et al.*, JCTC **13** (4), 1616 (2017), [4] V. Rokaj *et al.*, J. Phys. B **51**, 034005 (2018), [5] C. Schäfer *et al.*, in preparation (2019)

Limitations of models and standard approximations[3,4,5]



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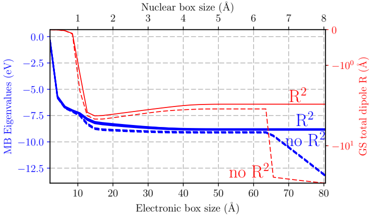

$\mathbf{R}\cdot\boldsymbol{\lambda}(\hat{a}+\hat{a}^\dagger)$ (dashed), $\mathbf{R}\cdot\left(\boldsymbol{\lambda}(\hat{a}+\hat{a}^\dagger)+\mathbf{R}\right)$ (solid)

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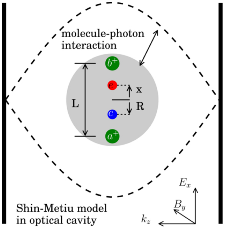

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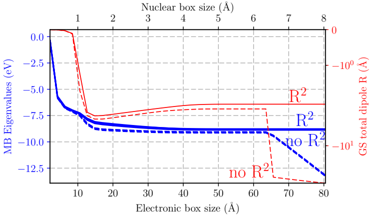
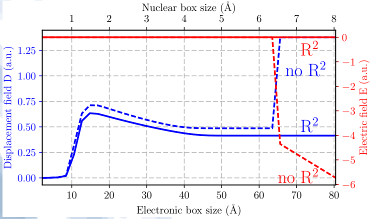


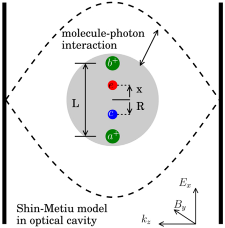
$\mathbf{R} \cdot \boldsymbol{\lambda}(\hat{a} + \hat{a}^\dagger)$ (dashed), $\mathbf{R} \cdot \left(\boldsymbol{\lambda}(\hat{a} + \hat{a}^\dagger) + \mathbf{R}\right)$ (solid)

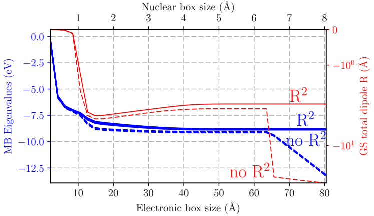


$\mathbf{D}_\perp = \boldsymbol{\lambda}(\hat{a} + \hat{a}^\dagger)$ and $\mathbf{E}_\perp = \left(\boldsymbol{\lambda}(\hat{a} + \hat{a}^\dagger) + \mathbf{R}\right)$

[3] J. Flick *et al.*, JCTC **13** (4), 1616 (2017), [4] V. Rokaj *et al.*, J. Phys. B **51**, 034005 (2018), [5] C. Schäfer *et al.*, in preparation (2019)

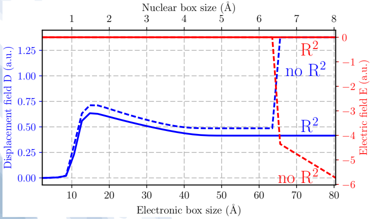
Limitations of models and standard approximations[3,4,5]

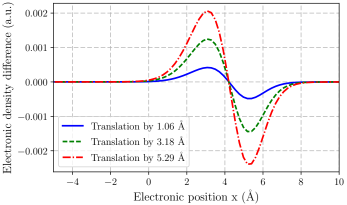




$\mathbf{R}\cdot\boldsymbol{\lambda}(\hat{a}+\hat{a}^\dagger)$ (dashed), $\mathbf{R}\cdot\left(\boldsymbol{\lambda}(\hat{a}+\hat{a}^\dagger)+\mathbf{R}\right)$ (solid)

Molecule (strong coupling).





$\mathbf{D}_\perp = \boldsymbol{\lambda}(\hat{a}+\hat{a}^\dagger)$ and $\mathbf{E}_\perp = \left(\boldsymbol{\lambda}(\hat{a}+\hat{a}^\dagger)+\mathbf{R}\right)$

[3] J. Flick *et al.*, JCTC **13** (4), 1616 (2017), [4] V. Rokaj *et al.*, J. Phys. B **51**, 034005 (2018), [5] C. Schäfer *et al.*, in preparation (2019)

Non-relativistic quantum-electrodynamics[6,7]

[6] D.P.Craig and T.Thirunamachandran, *Molecular QED*, Courier Corporation (1984)
[7] H.Spohn, *Dynamics of Charged Particles and their Radiation Field*, Cambridge University Press (2004)

Non-relativistic quantum-electrodynamics[6,7]

$$
\begin{aligned}
\hat{H}_{\mathrm{PF}}(t) = & \sum_{l=1}^{N_e} \frac{1}{2m}\left[\left(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{r}_l} + \frac{|e|}{c}\hat{\boldsymbol{A}}_{\perp}^{\mathrm{tot}}(\boldsymbol{r}_l,t)\right)\right]^2 + \frac{|e|\hbar}{2m}\boldsymbol{\sigma}_l \cdot \hat{\boldsymbol{B}}_{\perp}^{\mathrm{tot}}(\boldsymbol{r}_l,t) \\
& + \sum_{l=1}^{N_n} \frac{1}{2M_l}\left[\left(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{R}_l} - \frac{Z_l|e|}{c}\hat{\boldsymbol{A}}_{\perp}^{\mathrm{tot}}(\boldsymbol{R}_l,t)\right)\right]^2 - \frac{Z_l|e|\hbar}{2M_l}\boldsymbol{S}_l \cdot \hat{\boldsymbol{B}}_{\perp}^{\mathrm{tot}}(\boldsymbol{r}_l,t) \\
& + \frac{1}{2}\sum_{l\neq m}^{N_e} w(|\boldsymbol{r}_l - \boldsymbol{r}_k|) + \frac{1}{2}\sum_{l\neq m}^{N_n} Z_l Z_m w(|\boldsymbol{R}_l - \boldsymbol{R}_k|) \\
& - \sum_{l}^{N_e}\sum_{m}^{N_n} Z_m w(|\boldsymbol{r}_l - \boldsymbol{R}_m|) + \sum_{\boldsymbol{k},\lambda} \hbar\omega_k \hat{a}^{\dagger}_{\boldsymbol{k},\lambda}\hat{a}_{\boldsymbol{k},\lambda},
\end{aligned}
$$

[6] D.P.Craig and T.Thirunamachandran, *Molecular QED*, Courier Corporation (1984)
[7] H.Spohn, *Dynamics of Charged Particles and their Radiation Field*, Cambridge University Press (2004)

Non-relativistic quantum-electrodynamics[6,7]

mpsd

$$\hat{H}_{\mathrm{PF}}(t) = \sum_{l=1}^{N_e} \frac{1}{2m}\left[\left(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{r}_l} + \frac{|e|}{c}\hat{\boldsymbol{A}}_{\perp}^{\mathrm{tot}}(\boldsymbol{r}_l, t)\right)\right]^2 + \frac{|e|\hbar}{2m}\boldsymbol{\sigma}_l \cdot \hat{\boldsymbol{B}}_{\perp}^{\mathrm{tot}}(\boldsymbol{r}_l, t)$$

$$+ \sum_{l=1}^{N_n} \frac{1}{2M_l}\left[\left(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{R}_l} - \frac{Z_l|e|}{c}\hat{\boldsymbol{A}}_{\perp}^{\mathrm{tot}}(\boldsymbol{R}_l, t)\right)\right]^2 - \frac{Z_l|e|\hbar}{2M_l}\boldsymbol{S}_l \cdot \hat{\boldsymbol{B}}_{\perp}^{\mathrm{tot}}(\boldsymbol{r}_l, t)$$

$$+ \frac{1}{2}\sum_{l\neq m}^{N_e} w(|\boldsymbol{r}_l - \boldsymbol{r}_k|) + \frac{1}{2}\sum_{l\neq m}^{N_n} Z_l Z_m w(|\boldsymbol{R}_l - \boldsymbol{R}_k|)$$

$$- \sum_{l}^{N_e}\sum_{m}^{N_n} Z_m w(|\boldsymbol{r}_l - \boldsymbol{R}_m|) + \sum_{\boldsymbol{k},\lambda} \hbar\omega_k \hat{a}_{\boldsymbol{k},\lambda}^{\dagger}\hat{a}_{\boldsymbol{k},\lambda},$$

$$\hat{\boldsymbol{A}}_{\perp}^{\mathrm{tot}}(\boldsymbol{r}, t) = \hat{\boldsymbol{A}}_{\perp}(\boldsymbol{r}) + \boldsymbol{A}^{\mathrm{ext}}(\boldsymbol{r}, t), \quad \hat{\boldsymbol{B}}_{\perp}^{\mathrm{tot}}(\boldsymbol{r}, t) = \frac{1}{c}\boldsymbol{\nabla} \times \hat{\boldsymbol{A}}_{\perp}^{\mathrm{tot}}(\boldsymbol{r}, t)$$

$$w(|\boldsymbol{r} - \boldsymbol{r}'|) \overset{L\to\infty}{=} e^2/4\pi\epsilon_0|\boldsymbol{r} - \boldsymbol{r}'|$$

[6] D.P.Craig and T.Thirunamachandran, *Molecular QED*, Courier Corporation (1984)
[7] H.Spohn, *Dynamics of Charged Particles and their Radiation Field*, Cambridge University Press (2004)

Many-body methods for Pauli-Fierz field theory[8,9,10]

$$\hat{H}_{\mathrm{PF}}(t) = \hat{T} + \hat{W}(t) + \sum \hbar\omega_k \hat{a}^{\dagger}_{\boldsymbol{k},\lambda}\hat{a}_{\boldsymbol{k},\lambda} - \frac{1}{c}\int \mathrm{d}^3 r\ \hat{\boldsymbol{J}}(\boldsymbol{r},t)\cdot\hat{\boldsymbol{A}}^{\mathrm{tot}}_{\perp}(\boldsymbol{r},t)$$

Many-body methods for Pauli-Fierz field theory[8,9,10]

mpsd

$$\boxed{\hat{H}_{\mathrm{PF}}(t) = \hat{T} + \hat{W}(t) + \sum \hbar\omega_k \hat{a}^{\dagger}_{\boldsymbol{k},\lambda}\hat{a}_{\boldsymbol{k},\lambda} - \frac{1}{c}\int \mathrm{d}^3 r\ \hat{\boldsymbol{J}}(\boldsymbol{r},t)\cdot\hat{\boldsymbol{A}}^{\mathrm{tot}}_{\perp}(\boldsymbol{r},t)}$$

$$\hat{\boldsymbol{J}}(\boldsymbol{r},t) = \hat{\boldsymbol{j}}_{\mathrm{p}}(\mathbf{r}) + \hat{\boldsymbol{j}}_{\mathrm{m}}(\mathbf{r}) + \hat{\boldsymbol{A}}^{\mathrm{tot}}_{\perp}(\boldsymbol{r},t)\Bigg(\underbrace{\sum_{l=1}^{N_e}\frac{e^2}{mc}\,\delta(\mathbf{r}-\mathbf{r}_l)}_{=-\frac{|e|}{mc^2}\hat{n}_{\mathrm{e}}(\mathbf{r})} + \underbrace{\sum_{l=1}^{N_n}\frac{Z_l^2 e^2}{M_l c}\delta(\mathbf{r}-\boldsymbol{R}_l)}_{=\sum_n \frac{Z_n|e|}{M_n c^2}\hat{n}_n(\mathbf{r})}\Bigg),$$

$$\hat{\boldsymbol{j}}_{\mathrm{p}}(\mathbf{r}) = \sum_{l=1}^{N_e}\frac{|e|\hbar}{2m\mathrm{i}}\Big(\delta(\mathbf{r}-\mathbf{r}_l)\boldsymbol{\nabla}_{\mathbf{r}_l} - \overleftarrow{\boldsymbol{\nabla}}_{\mathbf{r}_l}\delta(\mathbf{r}-\mathbf{r}_l)\Big) + \sum_{l=1}^{N_n}\frac{Z_l|e|\hbar}{2M_l\mathrm{i}}\Big(\delta(\mathbf{r}-\boldsymbol{R}_l)\boldsymbol{\nabla}_{\boldsymbol{R}_l} - \overleftarrow{\boldsymbol{\nabla}}_{\boldsymbol{R}_l}\delta(\mathbf{r}-\boldsymbol{R}_l)\Big)$$

$$\hat{\boldsymbol{j}}_{\mathrm{m}}(\mathbf{r}) = \sum_{l=1}^{N_e}\frac{|e|\hbar}{2m}\boldsymbol{\nabla}_{\mathbf{r}_l}\times\left(\boldsymbol{\sigma}_l\delta(\mathbf{r}-\mathbf{r}_l)\right) - \sum_{l=1}^{N_n}\frac{Z_l|e|\hbar}{2M_l}\boldsymbol{\nabla}_{\boldsymbol{R}_l}\times\left(\boldsymbol{S}_l\delta(\mathbf{r}-\boldsymbol{R}_l)\right)$$

[8] M. Ruggenthaler *et al.*, PRA **90**, 012508 (2014), [9] M. Ruggenthaler *et al.*, Nat. Rev. Chem. **2**, 0118 (2018), [10] R. Jestädt *et al.*, arXiv:1812.05049 (2018)

Many-body methods for Pauli-Fierz field theory[8,9,10]

mpsd

$$\hat{H}_{\mathrm{PF}}(t) = \hat{T} + \hat{W}(t) + \sum \hbar\omega_k \hat{a}^{\dagger}_{\boldsymbol{k},\lambda}\hat{a}_{\boldsymbol{k},\lambda} - \frac{1}{c}\int \mathrm{d}^3r\, \hat{\boldsymbol{J}}(\boldsymbol{r},t)\cdot\hat{\boldsymbol{A}}^{\mathrm{tot}}_{\perp}(\boldsymbol{r},t)$$

$$\hat{\boldsymbol{J}}(\boldsymbol{r},t) = \hat{\boldsymbol{j}}_{\mathrm{p}}(\mathbf{r}) + \hat{\boldsymbol{j}}_{\mathrm{m}}(\mathbf{r}) + \hat{\boldsymbol{A}}^{\mathrm{tot}}_{\perp}(\boldsymbol{r},t)\Bigg(\underbrace{\sum_{l=1}^{N_e}\frac{e^2}{mc}\,\delta(\mathbf{r}-\mathbf{r}_l)}_{=-\frac{|e|}{mc^2}\hat{n}_{\mathrm{e}}(\mathbf{r})} + \underbrace{\sum_{l=1}^{N_n}\frac{Z_l^2 e^2}{M_l c}\delta(\mathbf{r}-\boldsymbol{R}_l)}_{=\sum_n \frac{Z_n|e|}{M_n c^2}\hat{n}_n(\mathbf{r})}\Bigg),$$

$$\hat{\boldsymbol{j}}_{\mathrm{p}}(\mathbf{r}) = \sum_{l=1}^{N_e}\frac{|e|\hbar}{2m\mathrm{i}}\Big(\delta(\mathbf{r}-\mathbf{r}_l)\boldsymbol{\nabla}_{\mathbf{r}_l} - \overleftarrow{\boldsymbol{\nabla}}_{\mathbf{r}_l}\delta(\mathbf{r}-\mathbf{r}_l)\Big) + \sum_{l=1}^{N_n}\frac{Z_l|e|\hbar}{2M_l\mathrm{i}}\Big(\delta(\mathbf{r}-\boldsymbol{R}_l)\boldsymbol{\nabla}_{\boldsymbol{R}_l} - \overleftarrow{\boldsymbol{\nabla}}_{\boldsymbol{R}_l}\delta(\mathbf{r}-\boldsymbol{R}_l)\Big)$$

$$\hat{\boldsymbol{j}}_{\mathrm{m}}(\mathbf{r}) = \sum_{l=1}^{N_e}\frac{|e|\hbar}{2m}\boldsymbol{\nabla}_{\mathbf{r}_l}\times\left(\boldsymbol{\sigma}_l\delta(\mathbf{r}-\mathbf{r}_l)\right) - \sum_{l=1}^{N_n}\frac{Z_l|e|\hbar}{2M_l}\boldsymbol{\nabla}_{\boldsymbol{R}_l}\times\left(\boldsymbol{S}_l\delta(\mathbf{r}-\boldsymbol{R}_l)\right)$$

- Density-functional theory for QED for $(\langle\hat{\boldsymbol{J}}\rangle, \langle\hat{\boldsymbol{A}}_{\perp}\rangle)$

[8] M. Ruggenthaler *et al.*, PRA **90**, 012508 (2014), [9] M. Ruggenthaler *et al.*, Nat. Rev. Chem. **2**, 0118 (2018), [10] R. Jestädt *et al.*, arXiv:1812.05049 (2018)

Many-body methods for Pauli-Fierz field theory[8,9,10]

mpsd

$$\hat{H}_{\mathrm{PF}}(t) = \hat{T} + \hat{W}(t) + \sum \hbar\omega_k \hat{a}^{\dagger}_{\boldsymbol{k},\lambda}\hat{a}_{\boldsymbol{k},\lambda} - \frac{1}{c}\int \mathrm{d}^3 r \; \hat{\boldsymbol{J}}(\boldsymbol{r},t)\cdot\hat{\boldsymbol{A}}^{\mathrm{tot}}_{\perp}(\boldsymbol{r},t)$$

$$\hat{\boldsymbol{J}}(\boldsymbol{r},t) = \hat{\boldsymbol{j}}_{\mathrm{p}}(\mathbf{r}) + \hat{\boldsymbol{j}}_{\mathrm{m}}(\mathbf{r}) + \hat{\boldsymbol{A}}^{\mathrm{tot}}_{\perp}(\boldsymbol{r},t)\Bigg(\underbrace{\sum_{l=1}^{N_e}\frac{e^2}{mc}\,\delta(\mathbf{r}-\mathbf{r}_l)}_{=-\frac{|e|}{mc^2}\hat{n}_{\mathrm{e}}(\mathbf{r})} + \underbrace{\sum_{l=1}^{N_n}\frac{Z_l^2 e^2}{M_l c}\delta(\mathbf{r}-\boldsymbol{R}_l)}_{=\sum_n \frac{Z_n|e|}{M_n c^2}\hat{n}_n(\mathbf{r})}\Bigg),$$

$$\hat{\boldsymbol{j}}_{\mathrm{p}}(\mathbf{r}) = \sum_{l=1}^{N_e}\frac{|e|\hbar}{2m\mathrm{i}}\Big(\delta(\mathbf{r}-\mathbf{r}_l)\boldsymbol{\nabla}_{\mathbf{r}_l} - \overleftarrow{\boldsymbol{\nabla}}_{\mathbf{r}_l}\delta(\mathbf{r}-\mathbf{r}_l)\Big) + \sum_{l=1}^{N_n}\frac{Z_l|e|\hbar}{2M_l\mathrm{i}}\Big(\delta(\mathbf{r}-\boldsymbol{R}_l)\boldsymbol{\nabla}_{\boldsymbol{R}_l} - \overleftarrow{\boldsymbol{\nabla}}_{\boldsymbol{R}_l}\delta(\mathbf{r}-\boldsymbol{R}_l)\Big)$$

$$\hat{\boldsymbol{j}}_{\mathrm{m}}(\mathbf{r}) = \sum_{l=1}^{N_e}\frac{|e|\hbar}{2m}\boldsymbol{\nabla}_{\mathbf{r}_l}\times\left(\boldsymbol{\sigma}_l\delta(\mathbf{r}-\mathbf{r}_l)\right) - \sum_{l=1}^{N_n}\frac{Z_l|e|\hbar}{2M_l}\boldsymbol{\nabla}_{\boldsymbol{R}_l}\times(\boldsymbol{S}_l\delta(\mathbf{r}-\boldsymbol{R}_l))$$

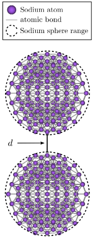
- Density-functional theory for QED for $(\langle\hat{\boldsymbol{J}}\rangle, \langle\hat{\boldsymbol{A}}_{\perp}\rangle)$
- Reduced density-matrix or Green's function theory

[8] M. Ruggenthaler *et al.*, PRA **90**, 012508 (2014), [9] M. Ruggenthaler *et al.*, Nat. Rev. Chem. **2**, 0118 (2018), [10] R. Jestädt *et al.*, arXiv:1812.05049 (2018)

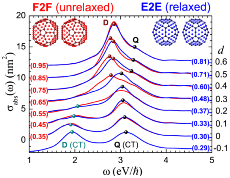
Quantum-electrodynamical density-functional simulation*

*see also poster 14. *Real-time solutions of coupled Ehrenfest-Maxwell-Pauli-Kohn-Sham equations: fundamentals, implementation, and nano-optical applications* by R. Jestädt

Quantum-electrodynamical density-functional simulation*



Nanoplasmonic dimer of two times 297 Sodium atoms and 297 valence electrons



The Journal of Physical Chemistry Letters, vol. 6, no. 10, pp. 1891-1898, (2015)

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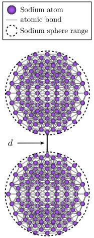

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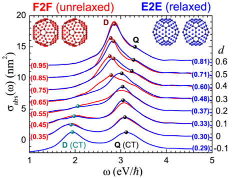
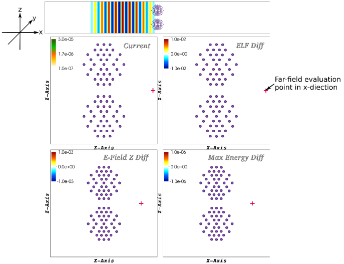


The Journal of Physical Chemistry Letters, vol. 6, no. 10, pp. 1891-1898, (2015)



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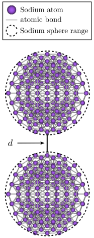
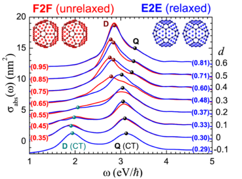
Quantum-electrodynamical density-functional simulation*

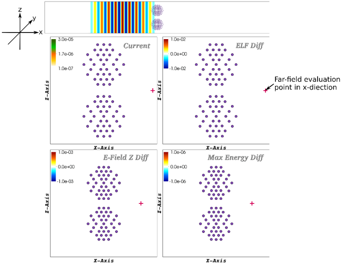
mpsd



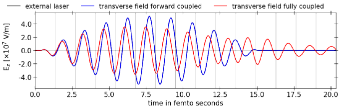
Nanoplasmonic dimer of two times 297 Sodium atoms and 297 valence electrons



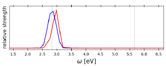
The Journal of Physical Chemistry Letters, vol. 6, no. 10, pp. 1891-1898, (2015)



Transverse electric field in z-direction and dipole approximation at the far-field point

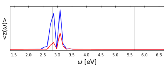


Fourier transform of E_z



Spectrum deduced from Maxwell

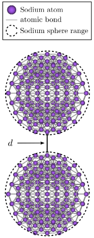
Fourier transform of $\langle z \rangle$



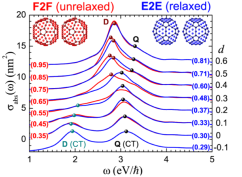
Spectrum deduced from matter

*see also poster 14. *Real-time solutions of coupled Ehrenfest-Maxwell-Pauli-Kohn-Sham equations: fundamentals, implementation, and nano-optical applications* by R. Jestädt

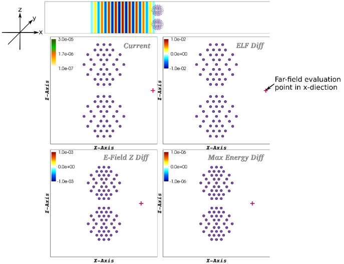
Quantum-electrodynamical density-functional simulation*



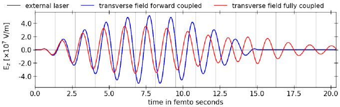
Nanoplasmonic dimer of two times 297 Sodium atoms and 297 valence electrons



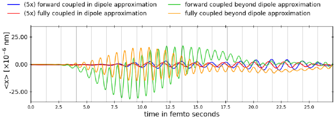
The Journal of Physical Chemistry Letters, vol. 6, no. 10, pp. 1891-1898, (2015)



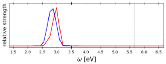
Transverse electric field in z-direction and dipole approximation at the far-field point



Dipole expectation value $\langle x \rangle$

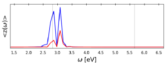


Fourier transform of E_z



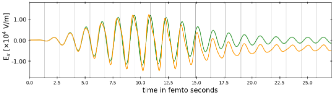
Spectrum deduced from Maxwell

Fourier transform of $\langle z \rangle$



Spectrum deduced from matter

x component of the electric field in at the far-field point in y-direction



*see also poster 14. *Real-time solutions of coupled Ehrenfest-Maxwell-Pauli-Kohn-Sham equations: fundamentals, implementation, and nano-optical applications* by R. Jestädt

Long-wavelength limit[1,4]

[1] C. Schäfer *et al.*, PRA **98**, 043801 (2018), [4] V. Rokaj *et al.*, J. Phys. B **51**, 034005 (2018)

Long-wavelength limit[1,4]

$$\hat{\boldsymbol{A}}_{\perp}(\boldsymbol{r}) \approx \hat{\boldsymbol{A}}_{\perp}(\boldsymbol{0}) \Rightarrow \int \mathrm{d}^3 r \, \hat{\boldsymbol{J}}(\boldsymbol{r}, t) \cdot \hat{\boldsymbol{A}}_{\perp}(\boldsymbol{0}, t) = \hat{\boldsymbol{R}} \cdot \hat{\boldsymbol{D}}$$

[1] C. Schäfer *et al.*, PRA **98**, 043801 (2018),[4] V. Rokaj *et al.*, J. Phys. B **51**, 034005 (2018)

Long-wavelength limit[1,4]

mpsd

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$\hat{\boldsymbol{R}} = \sum_l |e|(-\boldsymbol{r}_l + Z_l \boldsymbol{R}_l)$ and $\hat{\boldsymbol{D}} = \sum_{\boldsymbol{k},\lambda} \boldsymbol{\epsilon}(\boldsymbol{k}, \lambda) \underbrace{\frac{1}{\sqrt{2\omega_k}} \left(\hat{a}_{\boldsymbol{k},\lambda} + \hat{a}^{\dagger}_{\boldsymbol{k},\lambda} \right)}_{= q_{\boldsymbol{k},\lambda}}$

[1] C. Schäfer *et al.*, PRA **98**, 043801 (2018),[4] V. Rokaj *et al.*, J. Phys. B **51**, 034005 (2018)

Long-wavelength limit[1,4]

mpsd

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$\hat{\boldsymbol{R}} = \sum_l |e|(-\boldsymbol{r}_l + Z_l \boldsymbol{R}_l)$ and $\hat{\boldsymbol{D}} = \sum_{\boldsymbol{k},\lambda} \epsilon(\boldsymbol{k},\lambda)\underbrace{\frac{1}{\sqrt{2\omega_k}}\left(\hat{a}_{\boldsymbol{k},\lambda} + \hat{a}^{\dagger}_{\boldsymbol{k},\lambda}\right)}_{=q_{\boldsymbol{k},\lambda}}$

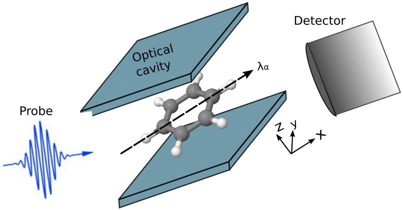
$$\boxed{\begin{aligned}\hat{H}(t) = &\hat{T} + \hat{W} + \sum \hbar\omega_k \hat{a}^{\dagger}_{\boldsymbol{k},\lambda}\hat{a}_{\boldsymbol{k},\lambda} - \hat{\boldsymbol{D}}\cdot\hat{\boldsymbol{R}} + \frac{1}{2}\sum_{\boldsymbol{k},\lambda}\left(\epsilon(\boldsymbol{k},\lambda)\cdot\hat{\boldsymbol{R}}\right)^2 \\ &+ \sum_l |e|\left(v(\boldsymbol{r}_l,t) - Z_l v(\boldsymbol{R}_l,t)\right)\end{aligned}}$$

[1] C. Schäfer *et al.*, PRA **98**, 043801 (2018), [4] V. Rokaj *et al.*, J. Phys. B **51**, 034005 (2018)

Cavity QED: ab-initio lifetimes and bath description[11]

[11] J. Flick *et al.*, arXiv:1803.02519 (2018)

Cavity QED: ab-initio lifetimes and bath description[11]



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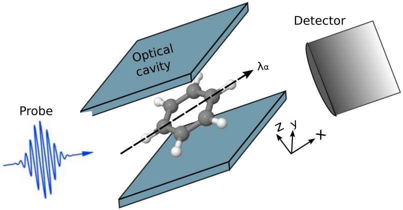

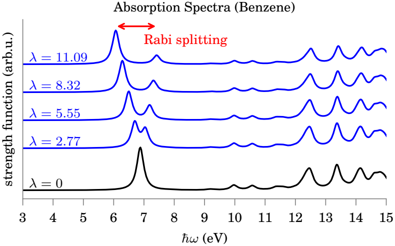

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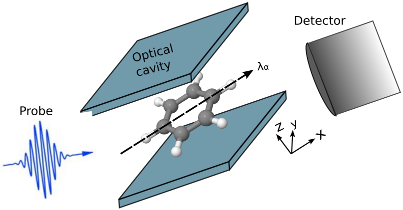

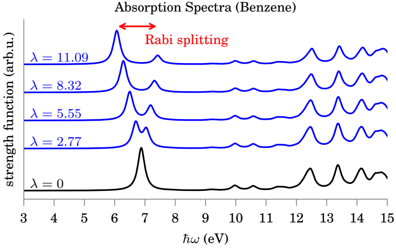

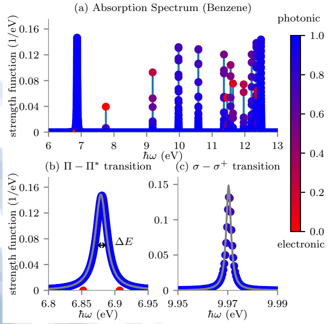

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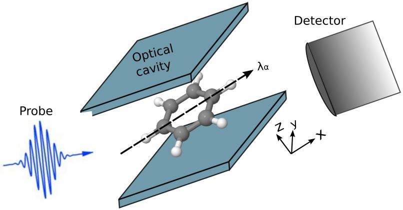

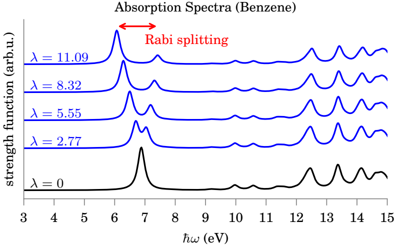

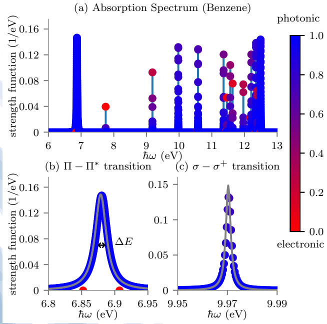

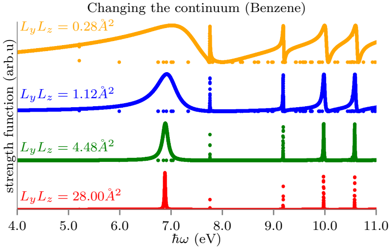

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Applications of ab-initio QED theory[†,12,13,14]

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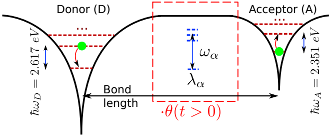

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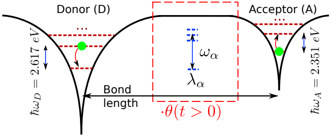

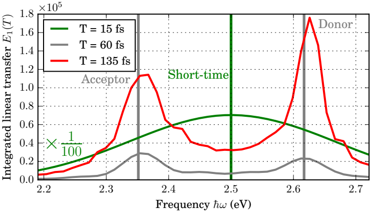

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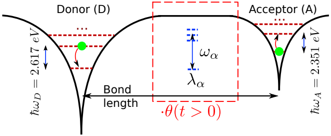

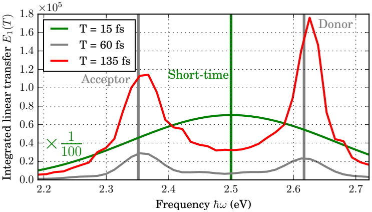

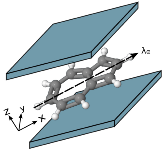

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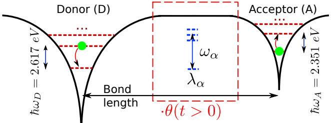

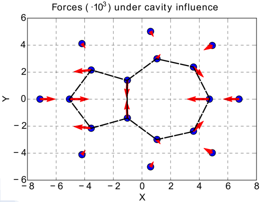

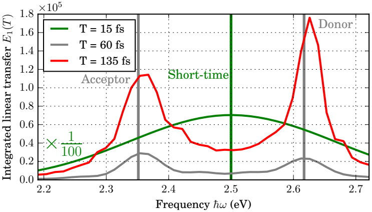

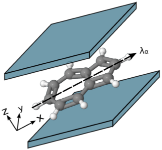

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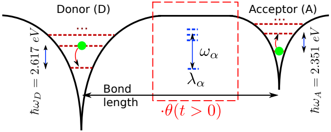

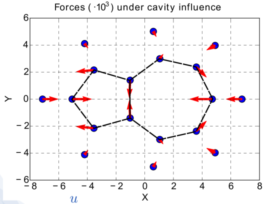

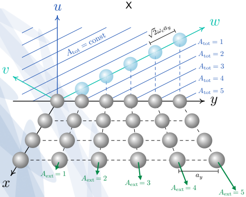

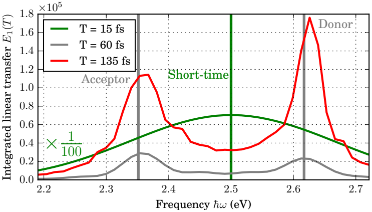

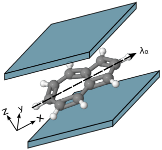

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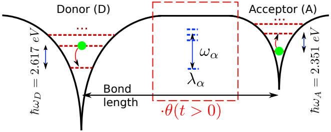

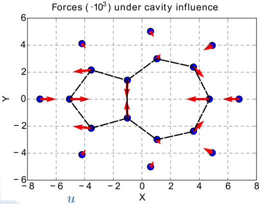

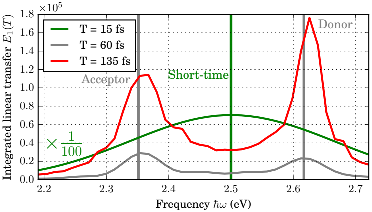

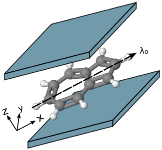

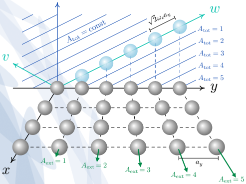

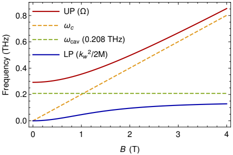

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Thank you for your Attention!

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Posters: **14.** *Real-time solutions of coupled Ehrenfest-Maxwell-Pauli-Kohn-Sham equations: fundamentals, implementation, and nano-optical applications* (R. Jestädt), **19.** *Modification of excitation and charge transfer in cavity quantum-electrodynamical chemistry* (C. Schäfer)