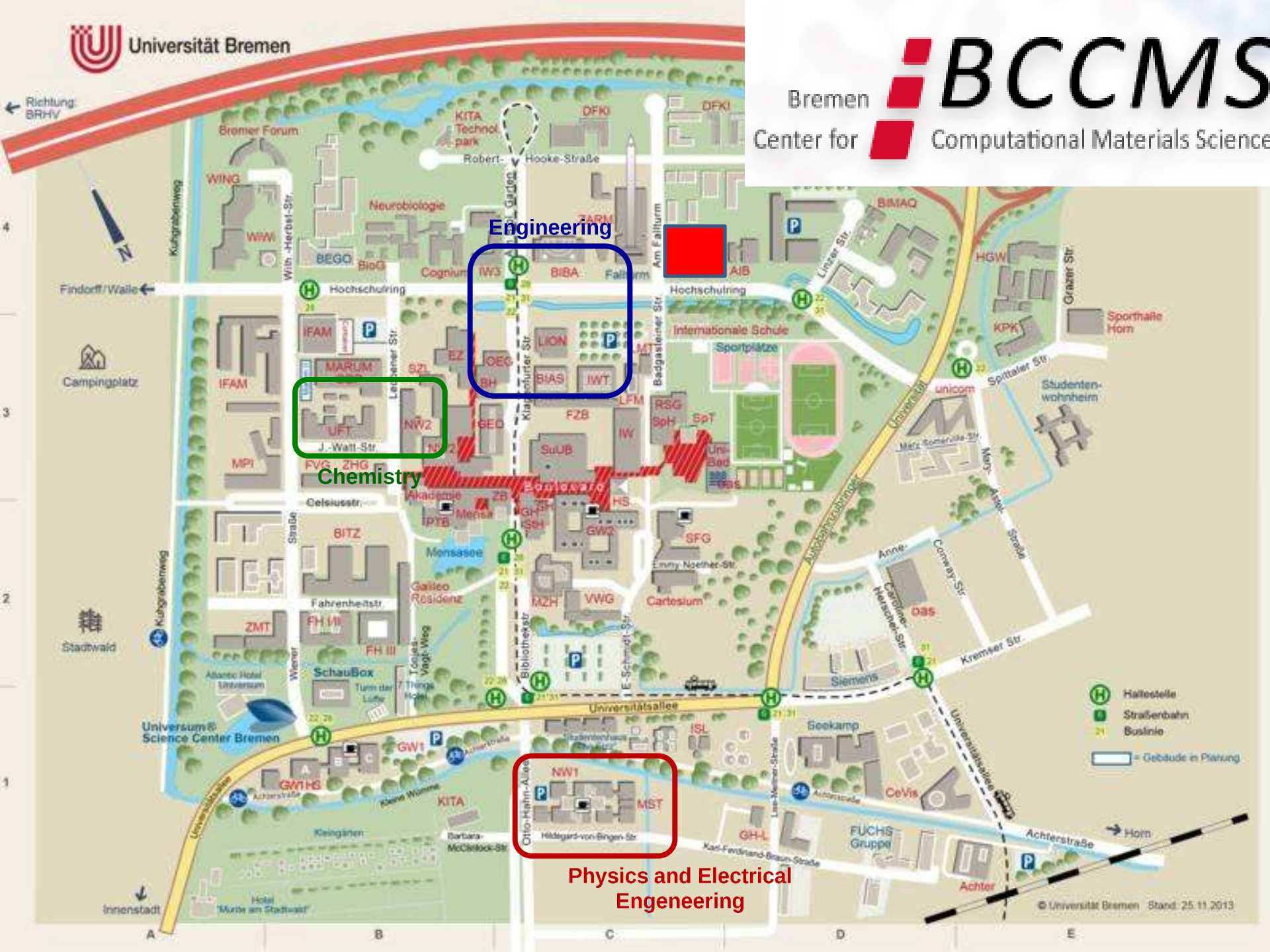
Bremen Center for Computational Materials Science


Universität Bremen
Bremen Center for BCCMS Computational Materials Science
Engineering
Chemistry
Physics and Electrical Engeneering
Richtung BRHV
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Campingplatz
Stadtwald
Innenstadt
Hochschulring
Celsiusstr.
Fahrenheitstr.
Universitätsallee
Kufsteiner Str.
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Buslinie
Gebäude in Planung
© Universität Bremen Stand: 25.11.2013

Bremen Center for Computational Materials Science

http://www.bccms.uni-bremen.de/

Founding Chair - 2006
Computational Materials Science

Thomas Frauenheim

Vasily Ploshikhin

Conrad-Naber Endowed Chair - 2008
Hybrid Materials Interfaces

Lucio Colombi Ciacchi

Airbus Endowed Chair – 2009/2010
Integrative Materials and Process Simulation & Engineering

Tim Wehling

Electronic Structure and Correlated Nanosystems – ECN 2012

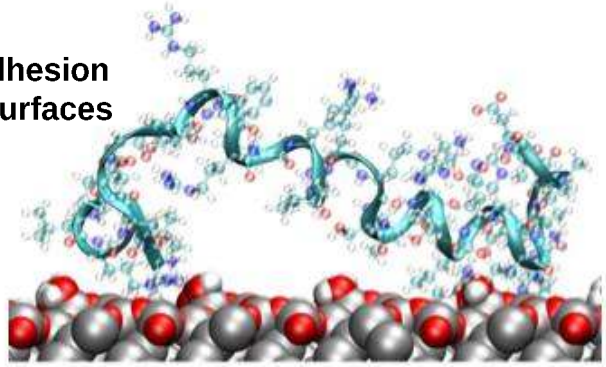
BCCMS

Bremen Center for Computational Materials Science

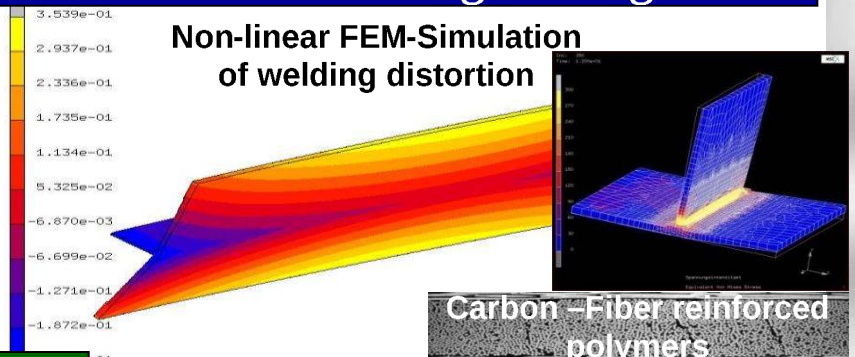
http://www.bccms.uni-bremen.de

Integrative Materials and Process Simulation & Engineering

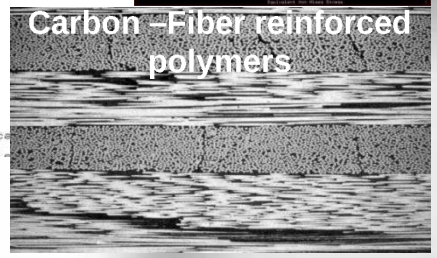
Collagen adhesion on silicon surfaces



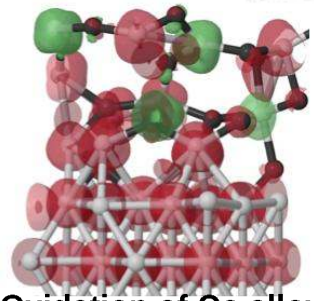
Non-linear FEM-Simulation of welding distortion



Carbon –Fiber reinforced polymers

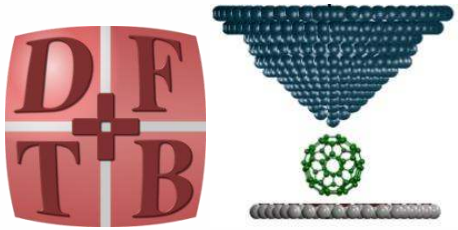


Hybrid Materials Interfaces

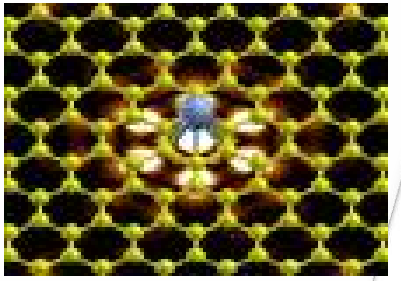


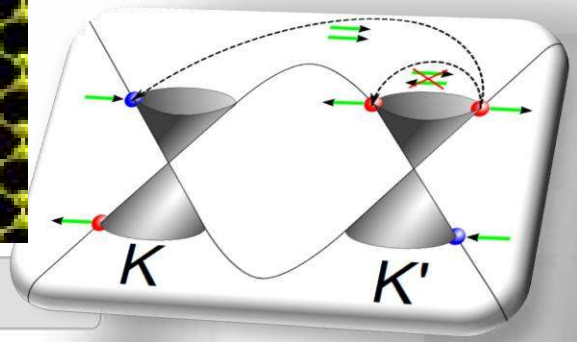
Oxidation of Co-alloys

Chemical reactive processes



ES & Correlated Nanosystems





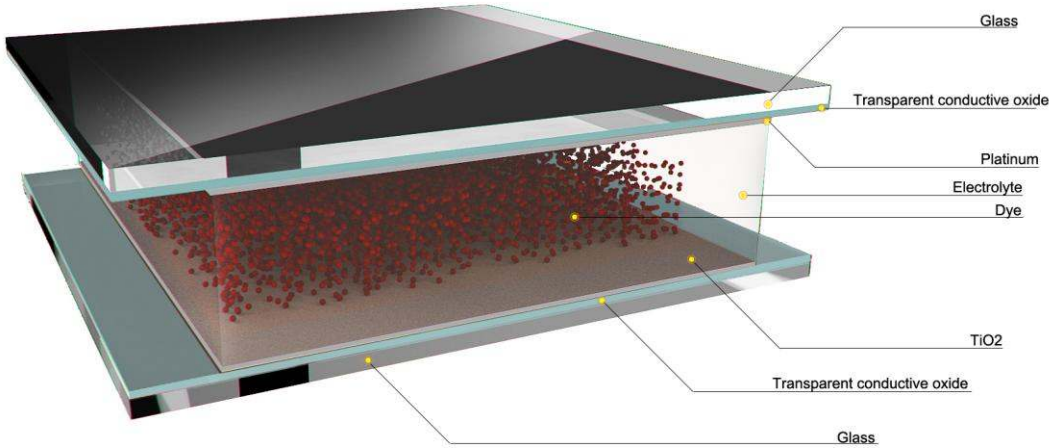
Computational Materials Science

BCCMS

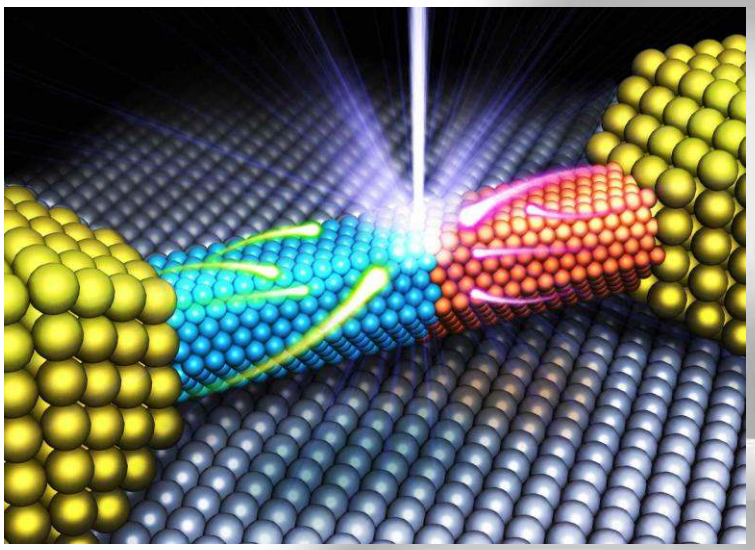
Physics of Graphene and novel layered materials/devices

Atomistic modeling of quantum processes in nanoscale devices

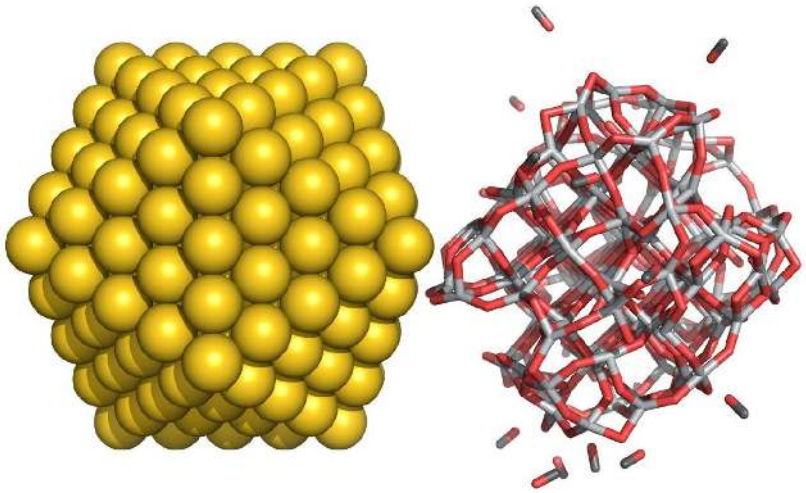
Photovoltaic devices



NW-LED



Hot electron injection



Solution of the many-body Schrödinger equation

$$\hat{H}\Psi(r_1, r_2, \ldots, r_N) = E\Psi(r_1, r_2, \ldots, r_N)$$

$$H_0 = T_{\mathrm{e}} + V_{\text{e-K}}(\underline{\mathbf{r}}, \underline{\mathbf{R}}) + V_{\text{e-e}}(\underline{\mathbf{r}}) + V_{\text{K-K}}(\underline{\mathbf{R}})$$

$$T_{\mathrm{e}} = \sum_{i=1}^{N_{\mathrm{e}}} \frac{\mathbf{p}_i^2}{2m} \qquad V_{\text{e-e}} = \sum_{i<j} v_{\text{e-e}}(\mathbf{r}_i - \mathbf{r}_j) \qquad v_{\text{e-e}}(\mathbf{r} - \mathbf{r}') = \frac{e^2}{|\mathbf{r} - \mathbf{r}'|}$$

Very challenging and expensive to solve directly though not impossible (for small systems)

Variational / diffusion Quantum Monte Carlo
Post-Hartree-Fock Quantum Chemistry

Density-Functional-Theory: DFT

For |GS> use density $n(r)$ instead of $\Psi(r_1, r_2, \ldots, r_N)$

$$E[\rho(\mathbf{r})] = \sum_{i=1}^{N} \int \psi_i(\mathbf{r}) \left(-\frac{\nabla^2}{2} \right) \psi_i(\mathbf{r})\, d\mathbf{r} + \frac{1}{2} \iint \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1\, d\mathbf{r}_2 + E_{XC}[\rho(\mathbf{r})]$$

$$- \sum_{A=1}^{M} \int \frac{Z_A}{|\mathbf{r} - \mathbf{R}_A|} \rho(\mathbf{r})\, d\mathbf{r}$$

$$E_H[\rho(\mathbf{r})] = \frac{1}{2} \iint \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{|r_1 - r_2|} d\mathbf{r}_1\, d\mathbf{r}_2$$

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} |\psi_i(\mathbf{r})|^2$$

$$E_{XC}[\rho(\mathbf{r})] = \int \rho(\mathbf{r}) \varepsilon_{XC}(\rho(\mathbf{r}))\, d\mathbf{r}$$

Includes all many-body effects

Kohn-Sham equation

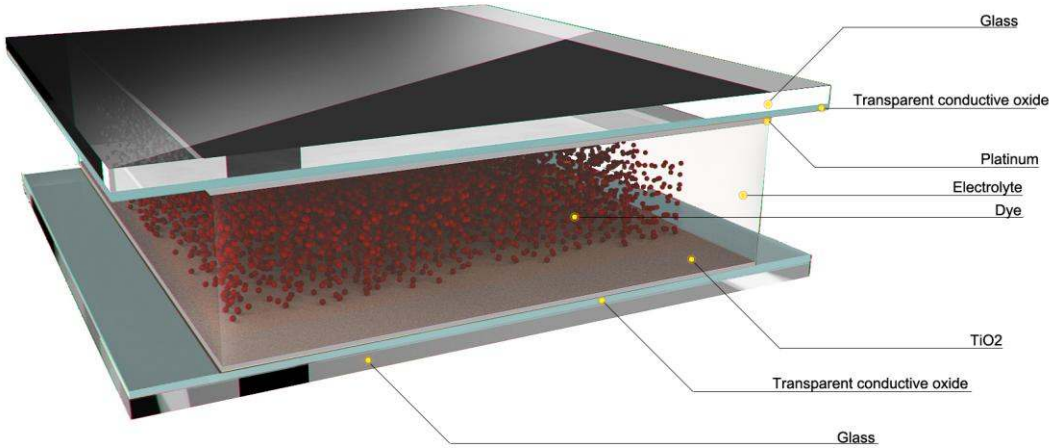
$$\left\{ -\frac{\nabla_1^2}{2} - \left(\sum_{A=1}^{M} \frac{Z_A}{r_{1A}} \right) + \int \frac{\rho(\mathbf{r}_2)}{r_{12}} d\mathbf{r}_2 + V_{XC}[\mathbf{r}_1] \right\} \psi_i(\mathbf{r}_1) = \varepsilon_i \psi_i(\mathbf{r}_1)$$

$$V_{XC}[\mathbf{r}] = \left(\frac{\delta E_{XC}[\rho(\mathbf{r})]}{\delta \rho(\mathbf{r})} \right)$$

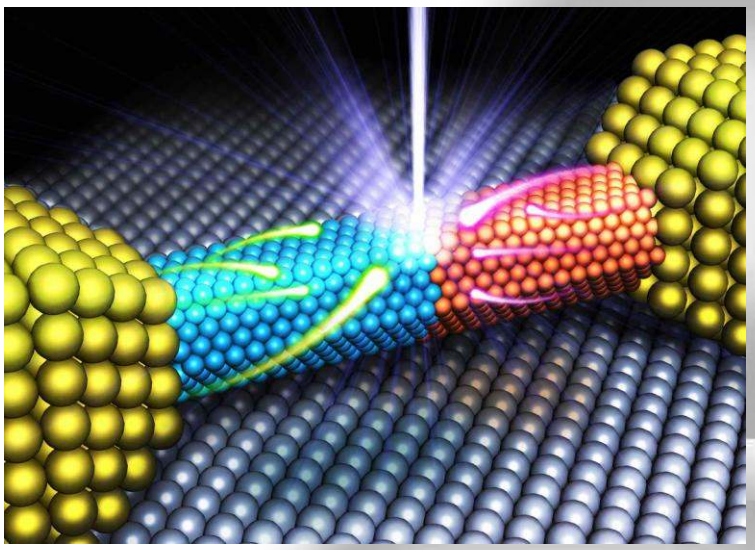
Today can be solved self-consitently for several 100 atoms

Atomistic modeling of quantum processes in nanoscale devices

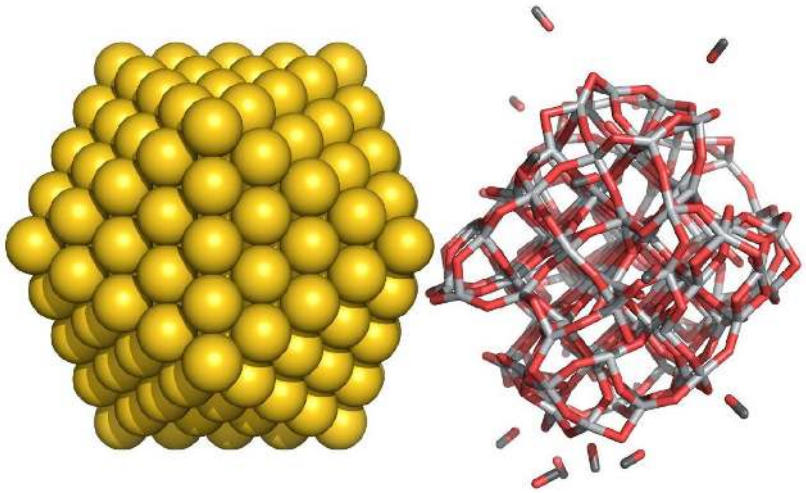
Photovoltaic devices



NW-LED

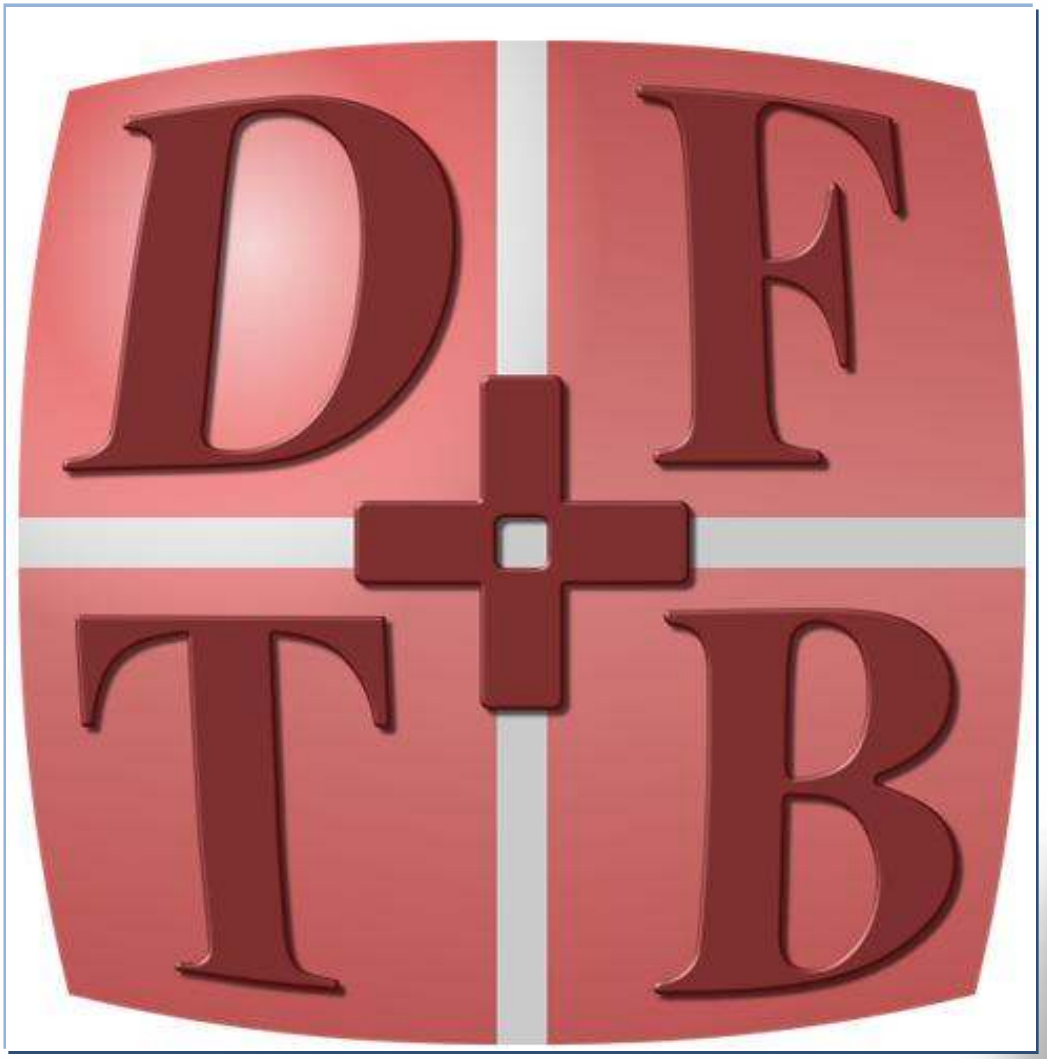


Hot electron injection



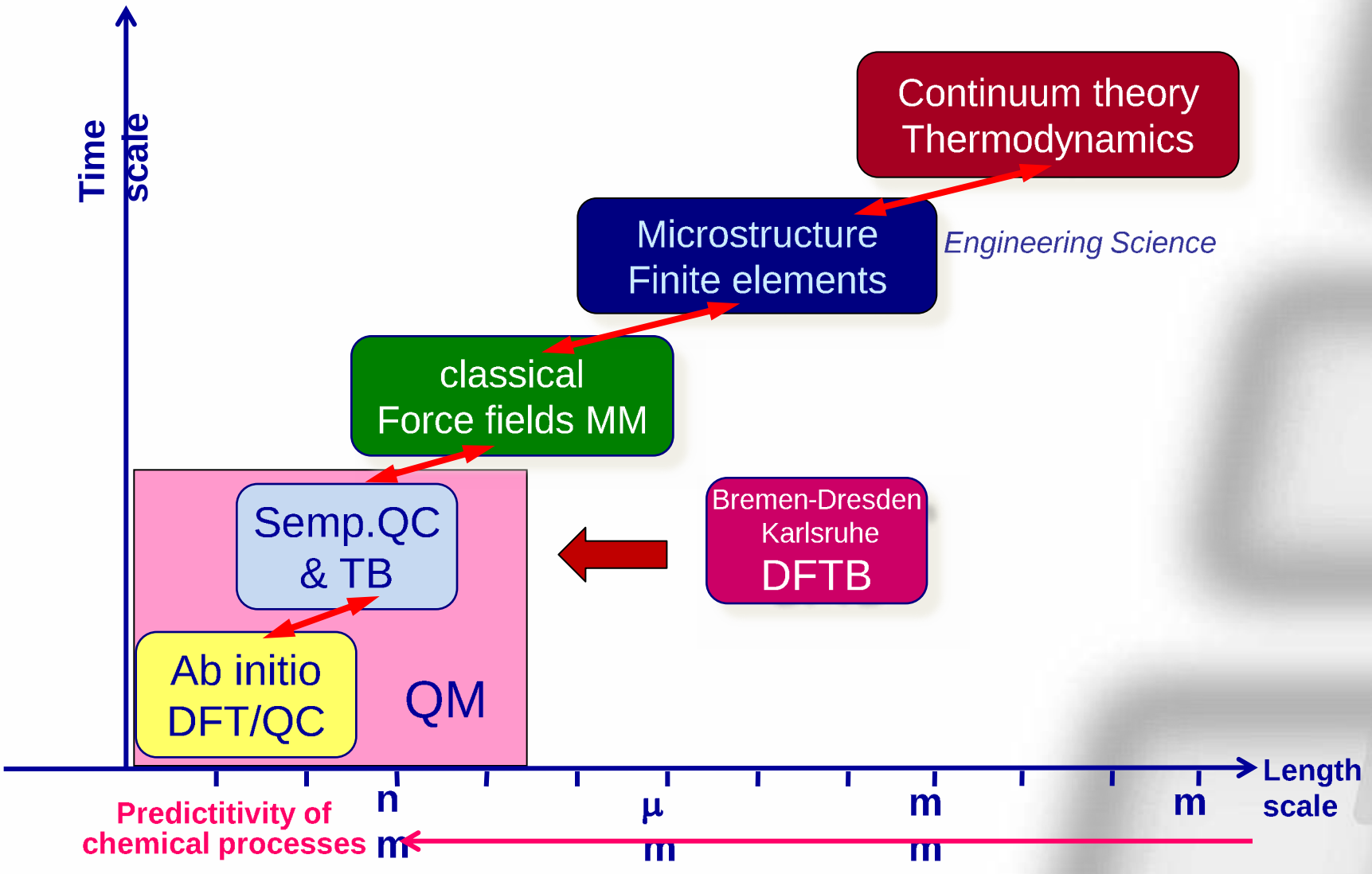
We need to go beyond 10.000 atom simulations

Atomistic modeling of photo-induced processes and energy conversion in nanoscale devices

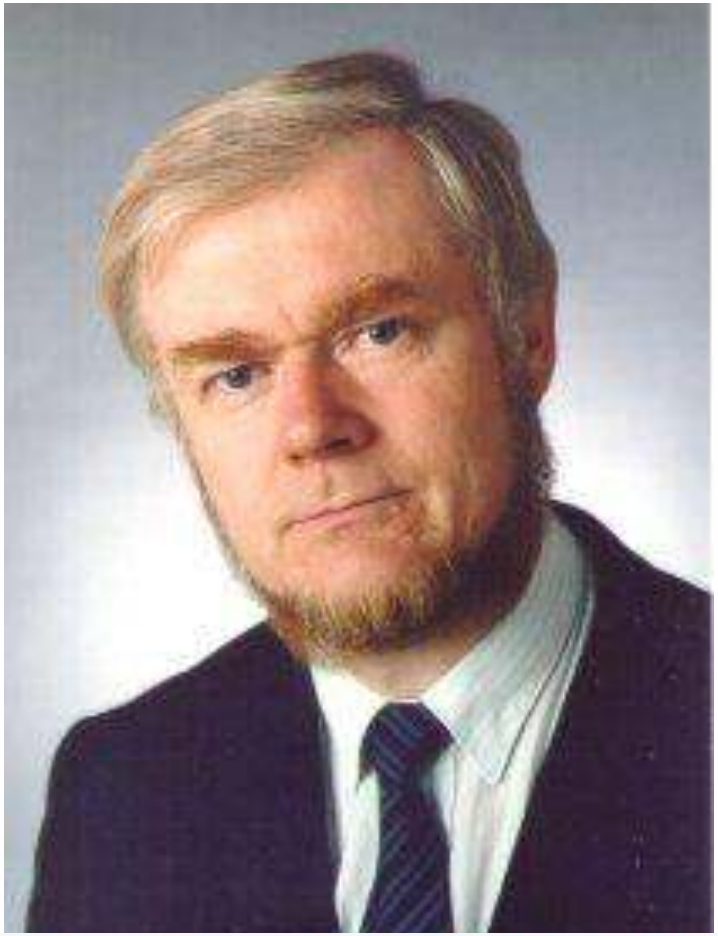


BCCMS

Multi-scale hierarchy in materials simulations



From the LCAO-X_α –method to a modern DFTB-scheme



AN APPROXIMATION VARIANT OF LCAO-X-ALPHA METHODS

By: SEIFERT, G; ESCHRIG, H; BIEGER, W
ZEITSCHRIFT FUR PHYSIKALISCHE CHEMIE-LEIPZIG Volume: 267 Issue: 3 Pages: 529-539 Published: 1986

Volltext SuUB Bremen

Times Cited: 92
(from Web of Science Core Collection)

Usage Count

PHYSICAL REVIEW B VOLUME 51, NUMBER 19 15 MAY 1995-I

Construction of tight-binding-like potentials on the basis of density-functional theory: Application to carbon

D. Porezag,* Th. Frauenheim, and Th. Köhler
Technische Universität, Institut für Physik, Theoretische Physik III, D-09009 Chemnitz, Germany

G. Seifert and R. Kaschner
Technische Universität Dresden, Institut für Theoretische Physik, Mommsenstrasse
(Received 2 November 1994)

We present a density-functional-based scheme for determining the necess
mon nonorthogonal tight-binding (TB) models within the framework of the
atomic-orbitals formalism using the local-density approximation (LDA). B
center integrals the Hamiltonian and overlap matrix elements are calculate
densities and potentials rather than fitted to experimental data. We can de
for the C-C, C-H, and H-H Hamiltonian and overlap matrix elements. The
sive potential appearing in most TB models is fitted to self-consistent calcul
the LDA. The calculation of forces is easy and allows an application of the
dynamics simulations. Despite its extreme simplicity, the method is transfer
and hydrocarbon systems. The determination of equilibrium geometries, to
tional modes of carbon clusters, hydrocarbon molecules, and solid-state
yield results showing an overall good agreement with more sophisticated m

sired matrix elements. For that reason, we will refer to our method as a nonorthogonal DF-based TB scheme.

BCCMS

DFTB: 1410 citations

PHYSICAL REVIEW B VOLUME 58, NUMBER 11 15 SEPTEMBER 1998-I

Self-consistent-charge density-functional tight-binding method for simulations of complex materials properties

M. Elstner
Universität-GH, Paderborn, Fachbereich Physik, Theoretische Physik, D-33098 Paderborn, Germany
and Department of Molecular Biophysics, German Cancer Research Center, D-69120 Heidelberg, Germany

D. Porezag, G. Jungnickel, J. Elsner, M. Haugk, and Th. Frauenheim
Universität-GH, Paderborn, Fachbereich Physik, Theoretische Physik, D-33098 Paderborn, Germany

S. Suhai
Department of Molecular Biophysics, German Cancer Research Center, D-69120 Heidelberg, Germany

G. Seifert
nstitut für Theoretische Physik, Mommsenstrasse 13, D-01062 Dresden, Germany
1 9 September 1997; revised manuscript received 19 March 1998)

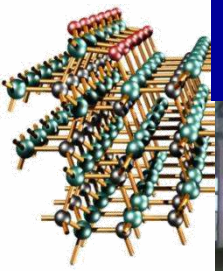
UPB Dr. habil 2003

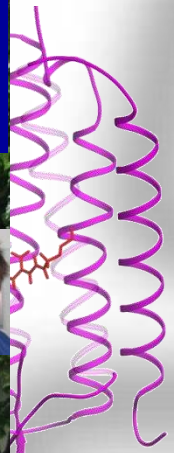
DFTB: 2562 citations

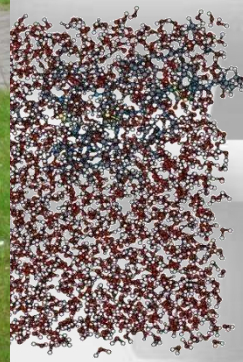
DFTB-method

Theory of complex materials @ UPB

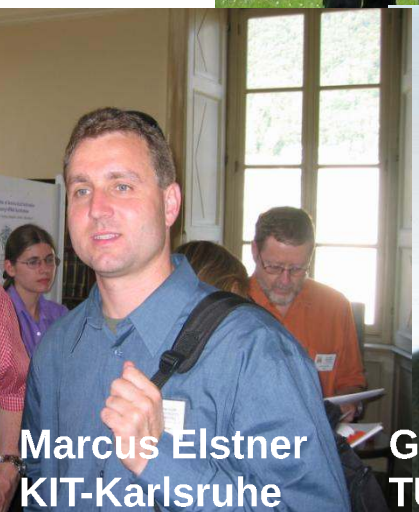
supported by DFG, DAAD, VW, EC, BMBF, FhG, Humboldt







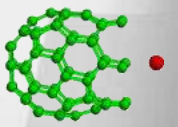
Collaborative effort



Marcus Elstner
KIT-Karlsruhe

Gotthard Seifert
TU Dresden

Theory of complex materials



Outline of the Talk

1. Brief introduction of the DFTB-method
2. Examples for device modeling
3. Ways to improve ground state accuracy and efficiency

4. TD-DFTB properties in linear response
5. NO-reduction on TiO_2 surfaces
6. Charge transfer exitations using pp-DFTB
7. Non-adiabatic Ehrenfest molecular dynamics

Outline of the Talk

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4. TD-DFTB properties in linear response
5. NO-reduction on TiO_2 surfaces
6. Charge transfer exitations using pp-DFTB
7. Non-adiabatic Ehrenfest molecular dynamics

DFTB relies on Density-Functional-Theory

For |GS> use density $n(r)$ instead of $\Psi(r_1, r_2, \ldots, r_N)$

$$E[\rho(\mathbf{r})] = \sum_{i=1}^{N} \int \psi_i(\mathbf{r}) \left(-\frac{\nabla^2}{2} \right) \psi_i(\mathbf{r})\, d\mathbf{r} + \frac{1}{2} \iint \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1\, d\mathbf{r}_2 + E_{XC}[\rho(\mathbf{r})]$$

$$- \sum_{A=1}^{M} \int \frac{Z_A}{|\mathbf{r} - \mathbf{R}_A|} \rho(\mathbf{r})\, d\mathbf{r}$$

$$E_H[\rho(\mathbf{r})] = \frac{1}{2} \iint \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{|r_1 - r_2|} d\mathbf{r}_1\, d\mathbf{r}_2$$

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} |\psi_i(\mathbf{r})|^2$$

$$E_{XC}[\rho(\mathbf{r})] = \int \rho(\mathbf{r}) \varepsilon_{XC}(\rho(\mathbf{r}))\, d\mathbf{r}$$

Includes all many-body effects

Kohn-Sham equation

$$\left\{ -\frac{\nabla_1^2}{2} - \left(\sum_{A=1}^{M} \frac{Z_A}{r_{1A}} \right) + \int \frac{\rho(\mathbf{r}_2)}{r_{12}} d\mathbf{r}_2 + V_{XC}[\mathbf{r}_1] \right\} \psi_i(\mathbf{r}_1) = \varepsilon_i \psi_i(\mathbf{r}_1)$$

$$V_{XC}[\mathbf{r}] = \left(\frac{\delta E_{XC}[\rho(\mathbf{r})]}{\delta \rho(\mathbf{r})} \right)$$

Today can be solved self-consitently for several 100 atoms

Major approximations in DFTB compared to DFT

- **Expansion of KSh-energy in 2nd or more recently 3rd order density fluctuation**
- **Reference density as atomic superposition** $n(\mathbf{r}) = n_0(\mathbf{r}) + \delta n(\mathbf{r}) \qquad n_0(\mathbf{r}) = \sum_\alpha n_0^\alpha(\mathbf{r} - \mathbf{R}_\alpha)$
- **Minimal basis representation of KSh-eigenstates** $\psi_i = \sum_\nu c_{i\nu}\,\phi(\mathbf{r} - \mathbf{R}_{\alpha(\nu)})$
- **Two-center integral approximation, fitting of repulsive interactions**
- **Self-consistency in atom-centered Mulliken charges in monopole approximation**

$$H^{\text{bs}}_{\mu\nu} = \langle \phi_\nu \,|\, \hat{T} + v_{\text{eff}}[n_0^\alpha + n_0^\beta] \,|\, \phi_\nu \rangle \qquad S_{\mu\nu} = \langle \phi_\mu \,|\, \phi_\nu \rangle$$

$$E^{\alpha\beta}_{\text{rep}}(R_{\alpha\beta}) = E_{\text{ab initio}}(R_{\alpha\beta}) - [E_{\text{bs}} + E_2](R_{\alpha\beta})$$

$$H^{\text{bs}}_{\mu\mu} = \varepsilon^{\text{free atom}}_{\mu}$$

What We NEED

- **H and S matrix versus distance for each At-type, At-type pair (s/p/d – 10 SK-tables)**
- **Automized tools will be made available – NEW SK-data format**

BCCMS

2-3 order of magnitude faster than DFT

http://www.dftb.org/

Go

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dftb.org the DFTB website

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Welcome to DFTB!

This site contains some information about the Density Fun
want to know more about this fast and efficient quantum m
short description about DFTB and eventually **some refer**

The DFTB method has several implementations. For a (n
implementations subpage.

If you are looking for parameters (Slater-Koster files), you c
and DFTB/Gaussian (soon).

accelrys
Materials studio

Many other worldwide distributed codes:
ADF, ATK, DeMon, CHARMM, Gaussian, ….

Three Slater-Koster sets available 2006-11-30

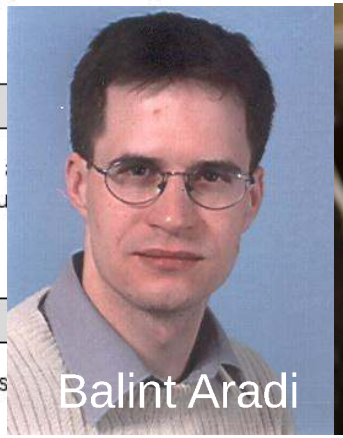
There are three Slater-Koster parameter sets (**mio-0-1**, **pbc-0-1**, **hyb-0-1**) available for **download**. They are provided by the groups of **Prof. Frauenheim** (**BCCMS**, Uni Bremen) and **Prof. Elstner** (**Theoretical Chemistry**, TU Braunschweig). With the help of these sets, the DFTB method can be applied to a broad range of systems, including organic and inorganic molecules, solid semiconductors and semiconductor surfaces and hybrid organic/inorganic systems.

DFTB+ on www.dftb-plus.info

The **dftb.org** site is being redesigned now. It should become a general site
distributing Slater-Koster parametrisation files for the method. Information abou
www.dftb-plus.info from now on.

DFTB at the ACS Fall Meeting in San Francisco (presentations)

The DFTB symposium at the ACS Fall Meeting in San Francisco was a real s
abstracts and some of the presentations are **available on our website** now.


Balint Aradi


Ben Hourahine

DFTB+ since 2007 distributed as open source code
about 3000 downloads

TB+ (Implemented/p

MM

M. Elstner, Q. Cui, M. Karplus

NEGreen-D

Charge trans

A. DiCarlo, A. P

Linear scalin

W. Yang

GW/BSE-DFTB

T. Niehaus

CPMD

T. Heine

LDA+U/SO

on-collin. magnetism

B. Hourahine

inter.

DFTB+

Since June: LGPL licenced open source DFTB+ release 17.1

We think its now time to go even further! The aim is to extend the active community and to make DFTB+ useful for an even broader scientific community in future years. Therefore, we have changed the license of the software to the open source license LGPL, enabling you to

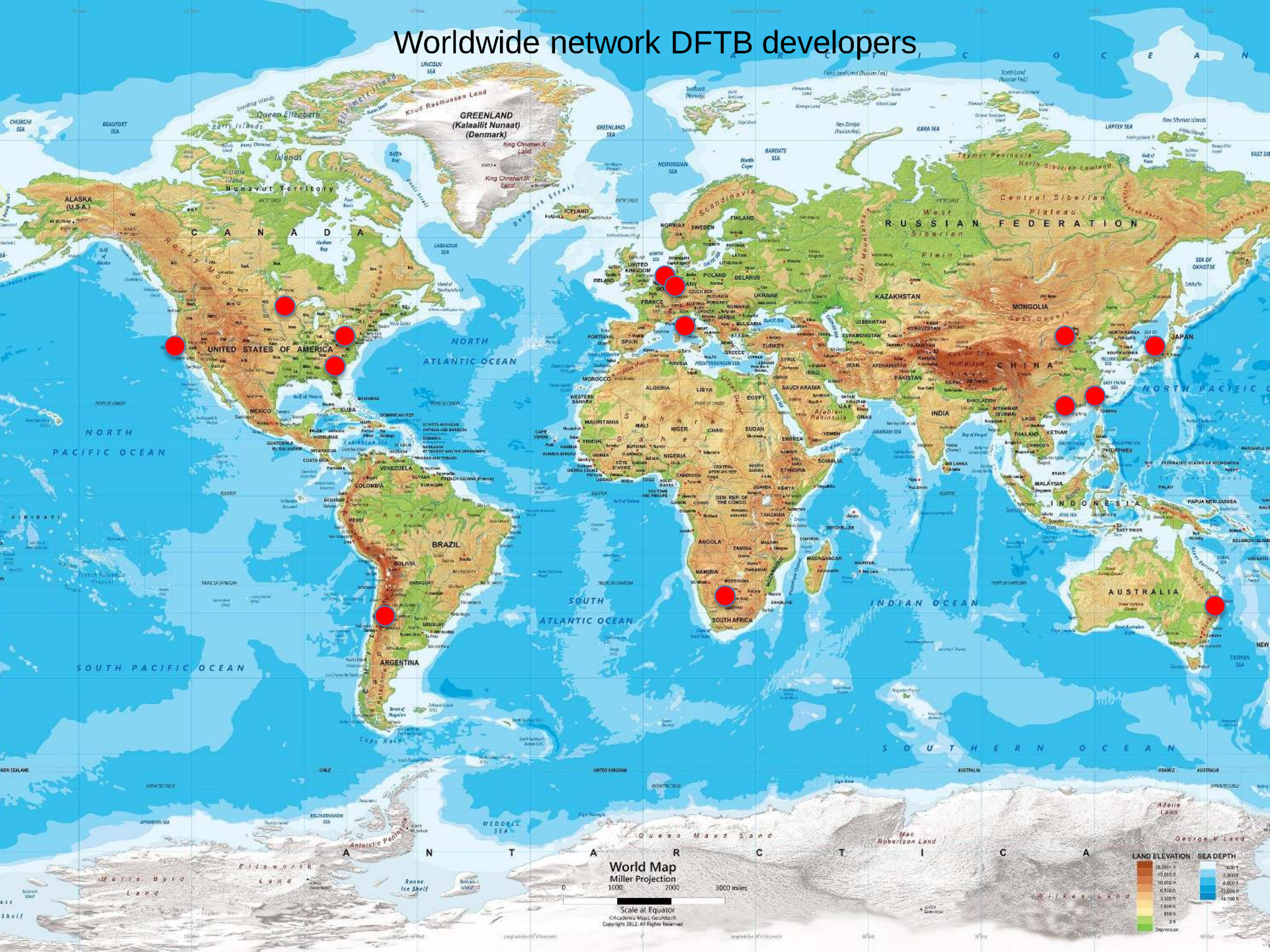
* obtain and use DFTB+ without any registration process, independent of whether your research is commercial or not,

* interface and distribute DFTB+ as part of your academic or commercial software package,

* easily contribute to DFTB+ by using our publicly hosted repository.

For more details see http://www.dftbplus.org

Worldwide network DFTB developers



DFTB Developer Meeting, October 2015

Next generation approximate DFTB method

cecam-MM1P.de

multi-scale modeling from first principles

DFTB Developer Meeting, November 2016

Next generation approximate DFTB method

cecam-MM1P.de multi-scale modeling from first principles

BEIJING COMPUTATIONAL SCIENCE RESEARCH CENTER

CSRC

English 简体中文

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International CECAM-Workshop on approximate quantum methods in the ab initio world

Objective : The primary goal of the proposed CECAM workshop is to facilitate communication and collaboration between users and developers of multi-scale quantum methods, with emphasis on approximate DFT and semi-empirical (SE) methods, linear-scaling quantum mechanical and hybrid quantum mechanical/molecular mechanics approaches. The meeting is intended to provide a unique forum to bring together world leaders of different communities in method development to discuss recent advances in current methodologies, to assess their similarities, and to identify critical challenges in the field as well as future directions for research and development of the next generation of computational tools. On the more technical side, this will include the discussion of the state of the art in efficient parameterization techniques, reference databases, and multi-objective optimization. Simultaneously, the workshop will involve people from the DFT and ab initio communities, who are interested in SE/DFTB methods as a supplement to their first principles codes, for example to use the more approximate quantum techniques for screening large numbers of structures in high-dimensional configuration space and for exploring extended trajectories under real environmental conditions (e.g. deMon2k, ATK, ADF, SIESTA).

Date : November 6-13,2016

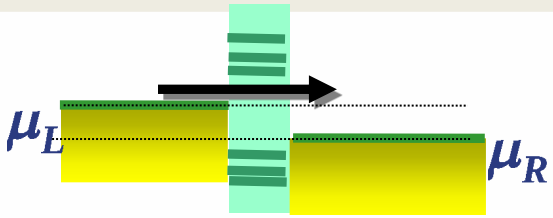
cecam

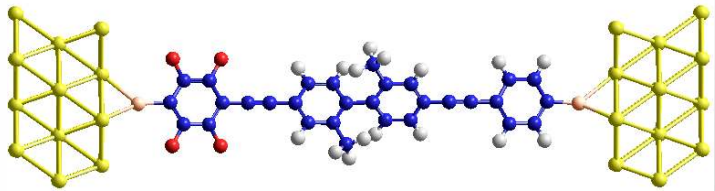
DFTB Developer Meeting in Telluride
23rd – 27th July 2018

cecam-MM1P.de
multi-scale modeling from first principles

Multi-Scale Quantum Mechanical Analysis of Condensed Phase Systems: Methods and Applications

NEGF quantum transport under open boundary conditions





$H^0_{\mu\nu}$

External potential + Hartree term + Exchange-correlation (LDA)

$H^1_{\mu\nu}$

Multigrid Poisson solver

Green's function

Δq_i

Self-consistent solutions

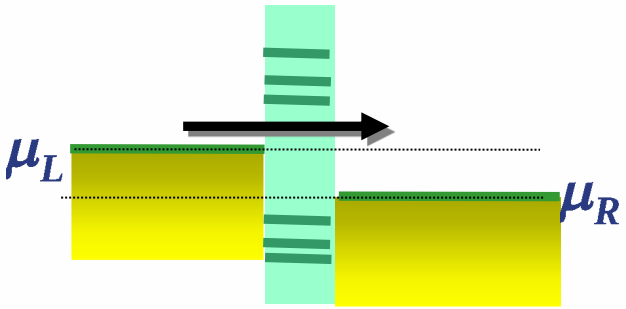
G^R e Σ^R

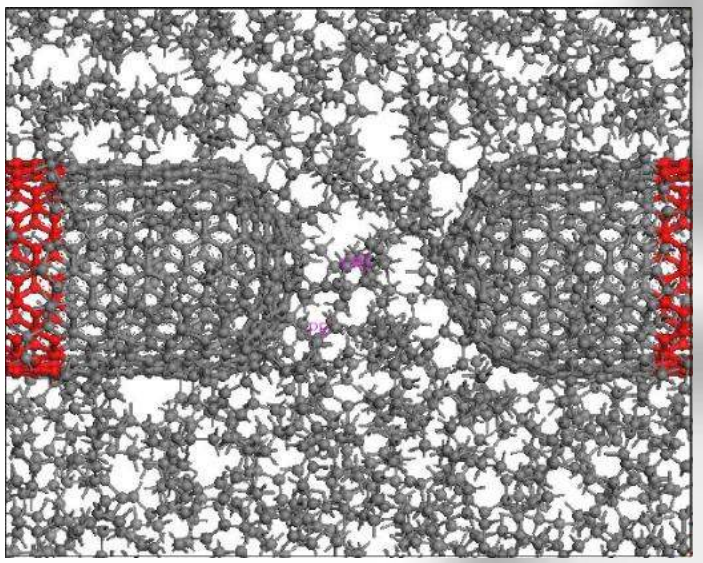
Density matrix ρ

$\int G^<$

Evaluation of $G^<$ $\Sigma^<$

Single molecule quantum transport



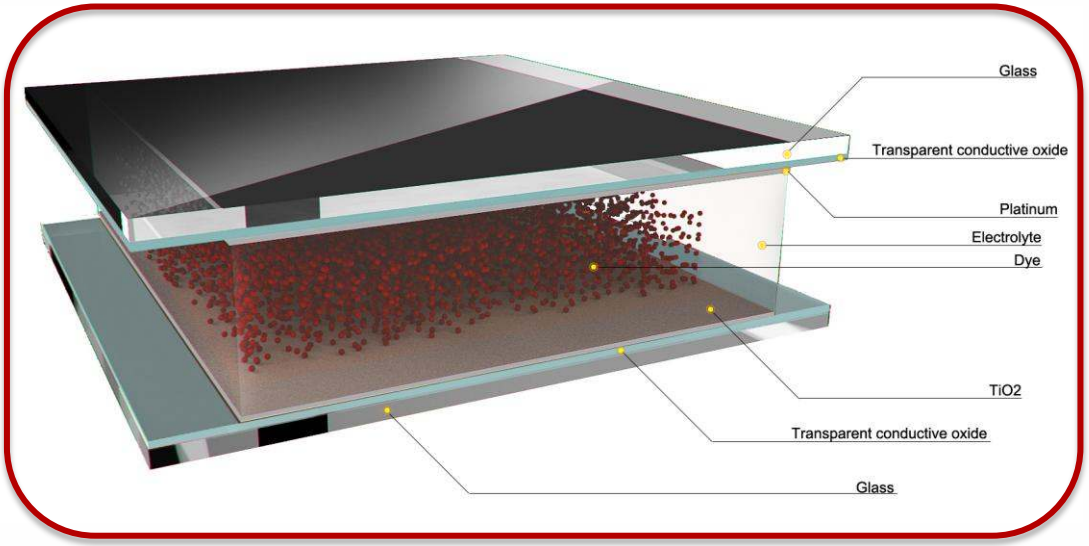


$$I = \frac{2e}{h}\int_{\mu_R}^{\mu_L} Tr[\Sigma^{<}G^{>} - \Sigma^{>}G^{<}]dE$$

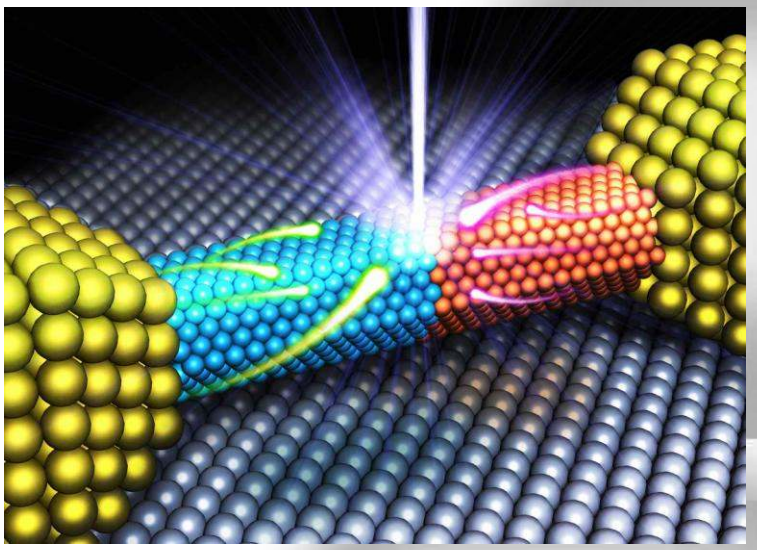
Meir & Wingreen, Phys. Rev. Lett. (1992)

Atomistic modeling of quantum processes in nanoscale devices

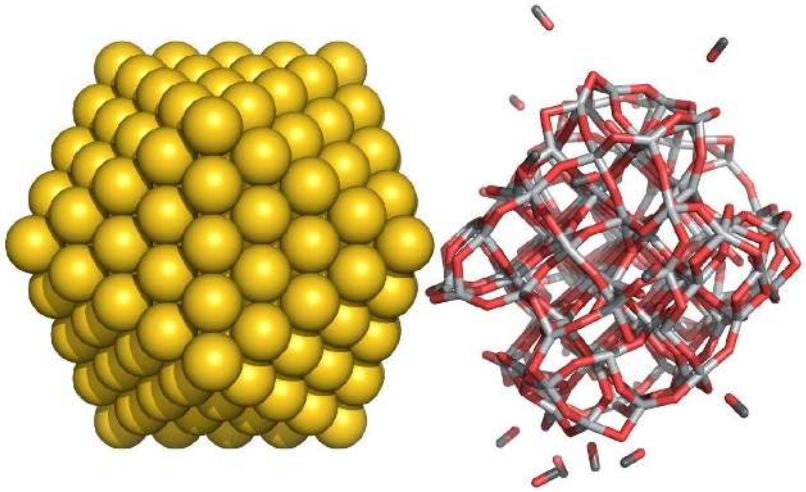
Photovoltaic devices



NW-LED



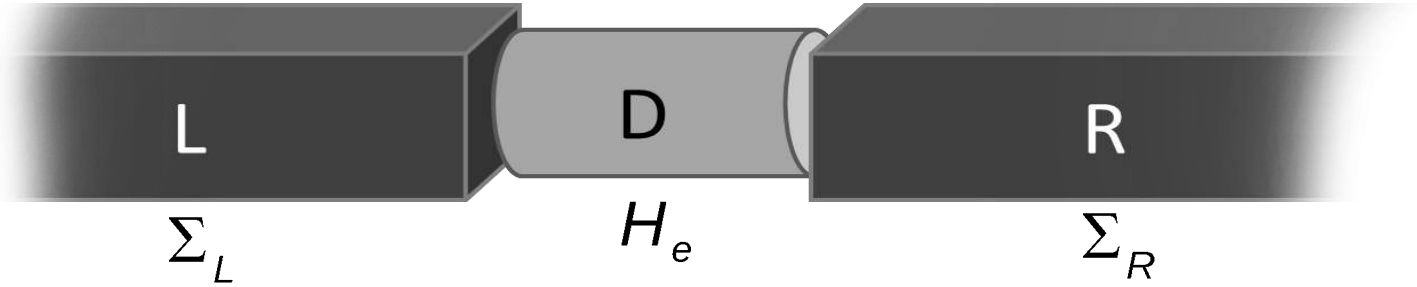
Hot electron injection



Electron – photon interaction

Electron-Photon Interactions

SiNW-SC PN-junction, linearly polarized light applied:



Hamiltonian in Coulomb Gauge:

$$H = \frac{1}{2m}(p + e\vec{A})^2 + V(\vec{r}) \equiv H_e + \frac{e}{m}\vec{A}\cdot\vec{p} + \frac{e^2}{2m}\vec{A}^2$$

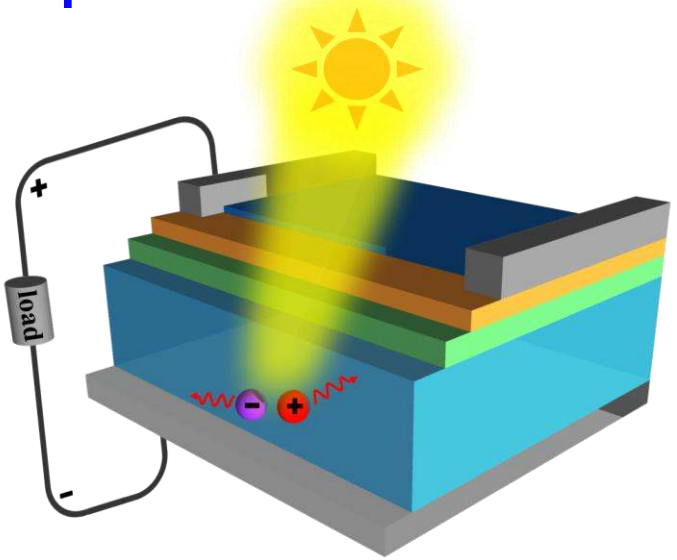
In dipole approximation - vector potential in **second quantization**:

$$\vec{A} = \vec{a}\left(\frac{\hbar\sqrt{\tilde{\mu}\tilde{\varepsilon}}}{2N\omega\varepsilon c}F_r\right)^{1/2}\left(be^{-i\omega t} + b^{\dagger}e^{i\omega t}\right)$$

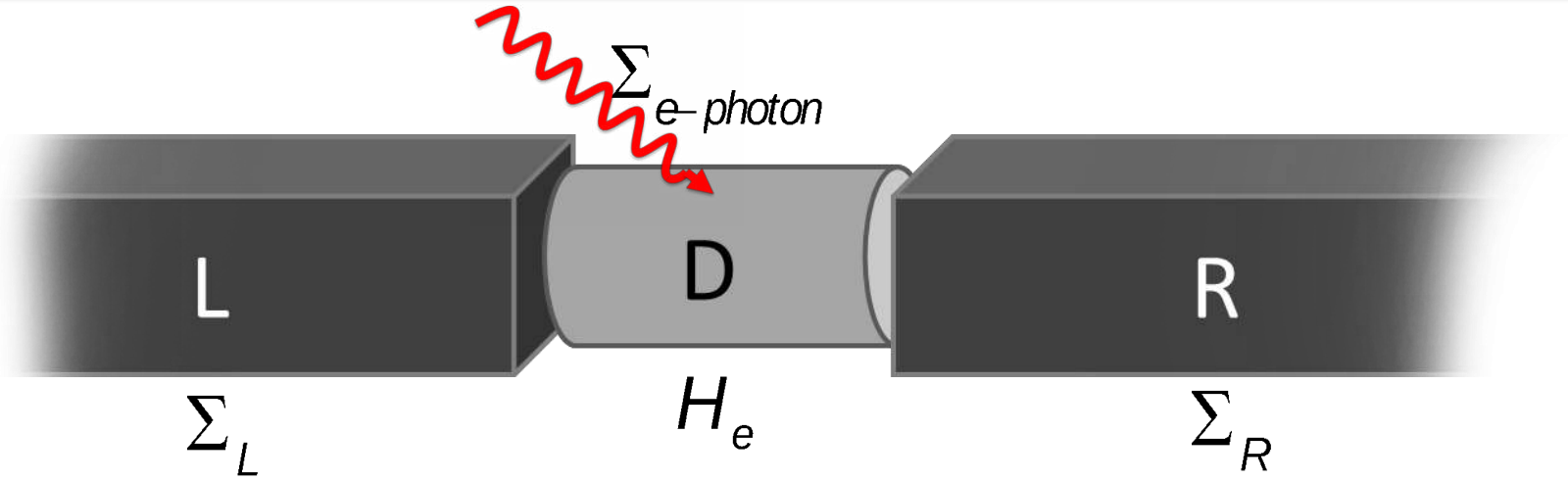
interaction Hamiltonian in atomic basis

$$H_{ep} = \sum_{\mu\nu}\frac{e}{m}\left\langle\mu\left|\vec{A}\cdot\vec{p}\right|\nu\right\rangle d_\mu^* d_\nu = \sum_{\mu\nu} M_{\mu\nu}(be^{-i\omega t} + b^* e^{i\omega t}) d_\mu^* d_\nu$$

very similar to electron-phonon interaction



Electron-Photon Interactions



$$\Sigma_{ep}(\tau,\tau') = iM[D(\tau,\tau')G(\tau,\tau')]M$$

Photon Green's Function: $D^{>}(t,t') = [Ne^{i\omega(t-t')} + (N+1)e^{-i\omega(t-t')}]$

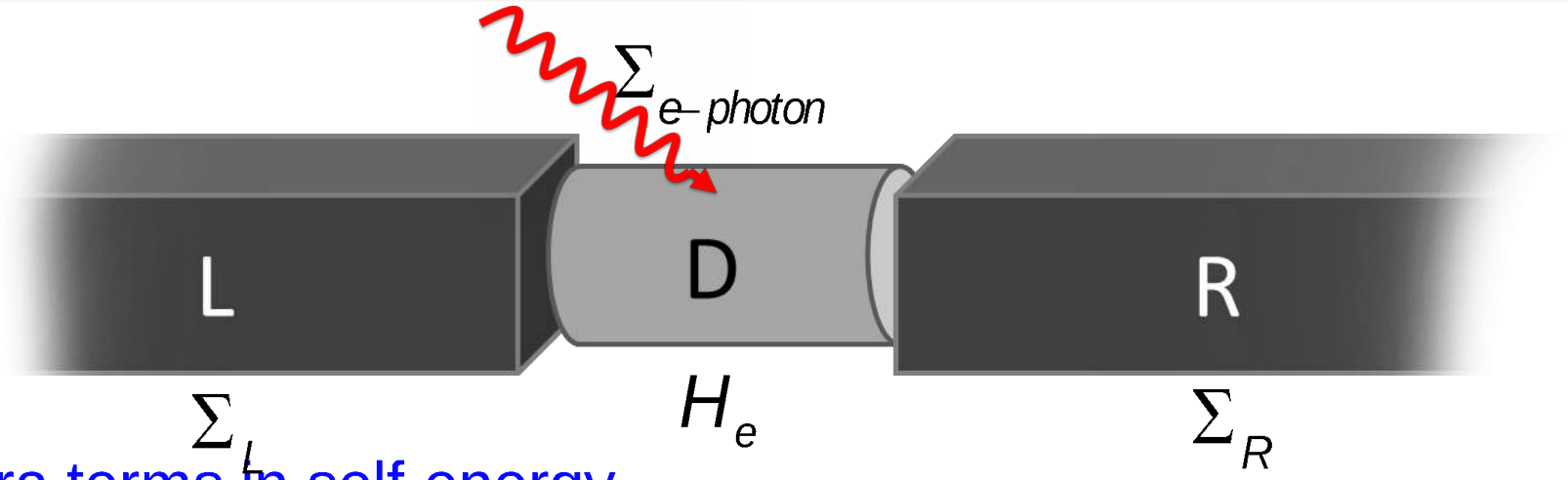
$$D^{<}(t,t') = [Ne^{-i\omega(t-t')} + (N+1)e^{i\omega(t-t')}]$$

Fourier transform:

$$\Sigma_{ep}^{<,>}(E) = M\left[\underset{\text{absorption}}{NG^{<,>}(E \mp \hbar\omega)} + \underset{\text{emission}}{(N+1)G^{<,>}(E \pm \hbar\omega)}\right]M$$

Both Green´s functions and self energies to be calculated self-consistentl

Electron-Photon Interactions



Extra terms in self-energy

$$G^r(E) = \left[ES - H - \Sigma_L^r(E) - \Sigma_R^r(E) - \Sigma_{ep}^r(E) \right]^{-1}$$

Current in NEGF:

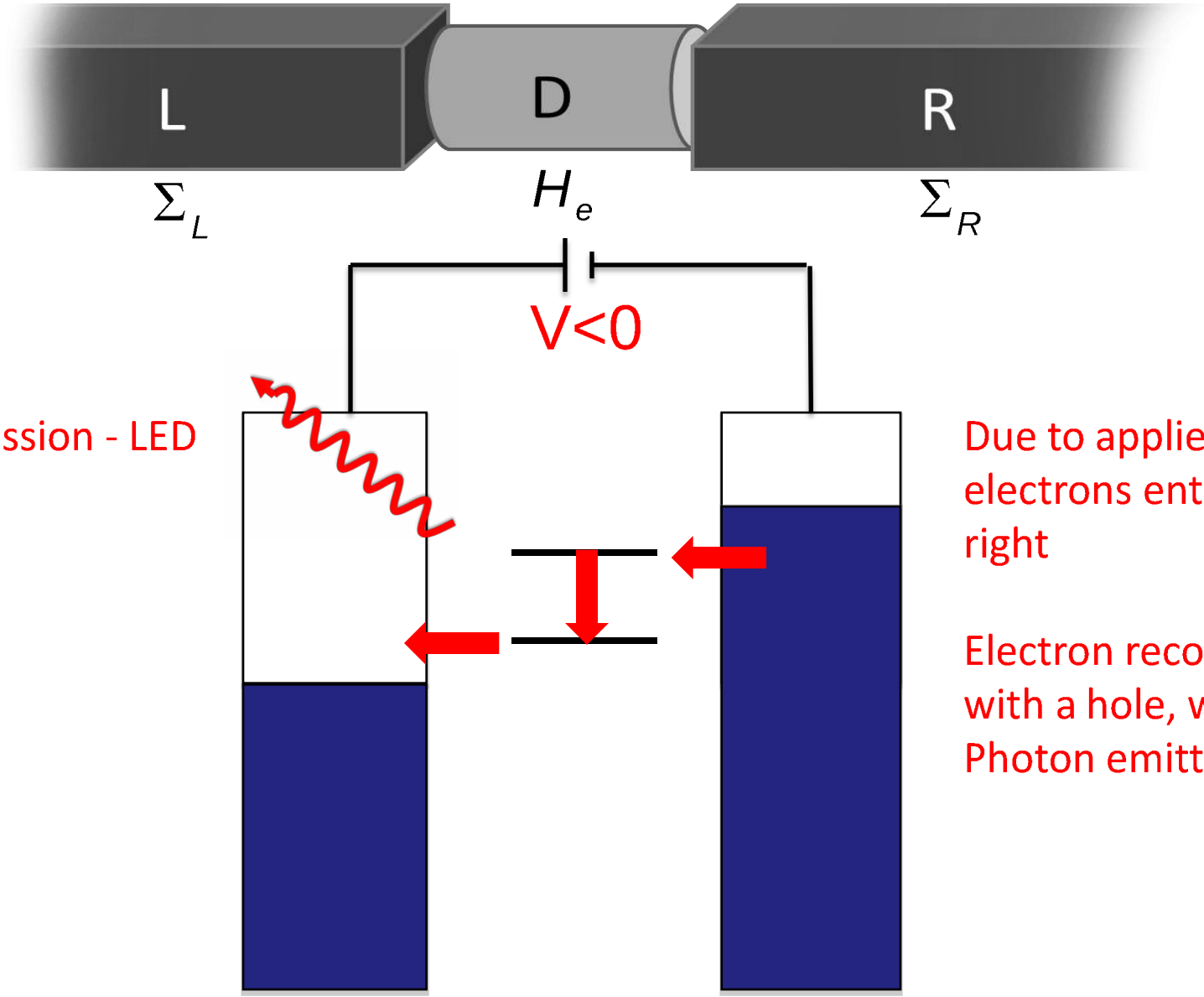
$$I_\alpha = \frac{2e}{\hbar} \int \frac{dE}{2\pi} \mathrm{Tr}\left[\Sigma_\alpha^<(E) G^>(E) - \Sigma_\alpha^>(E) G^<(E) \right]$$

Current:

- elastic part: $I_\alpha^{el} = \frac{2e}{\hbar} \int \frac{dE}{2\pi} \left(f_\alpha - f_\beta \right) \mathrm{Tr}\left[\Gamma_\alpha(E) G^r(E) \Gamma_\beta(E) G^a(E) \right]$
- inelastic part: $I_\alpha^{inel} = \frac{2e}{\hbar} \int \frac{dE}{2\pi} \mathrm{Tr}[\Gamma_\alpha(E) G^r(E) \Gamma_{eff}(E) G^a(E)]$

J. Phys. Chem. Lett. **5**, 1272 (201

Inelastic scatterings

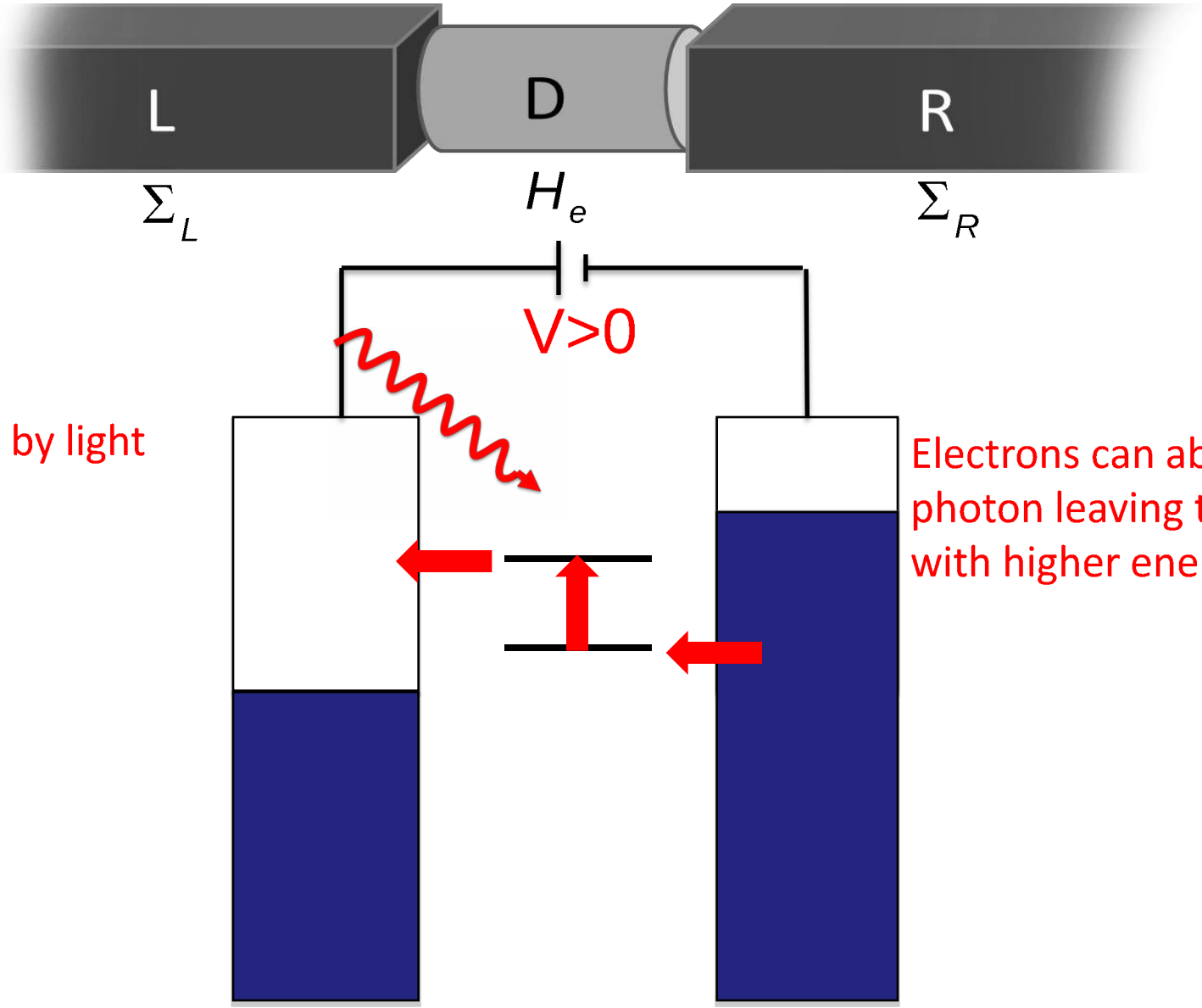


Light emission - LED

Due to applied bias electrons enter from right

Electron recombines with a hole, while a Photon emitted

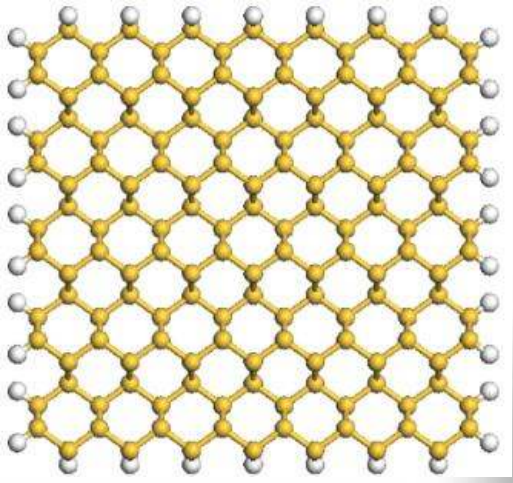
Inelastic scatterings



Excitation by light
Solar Cell

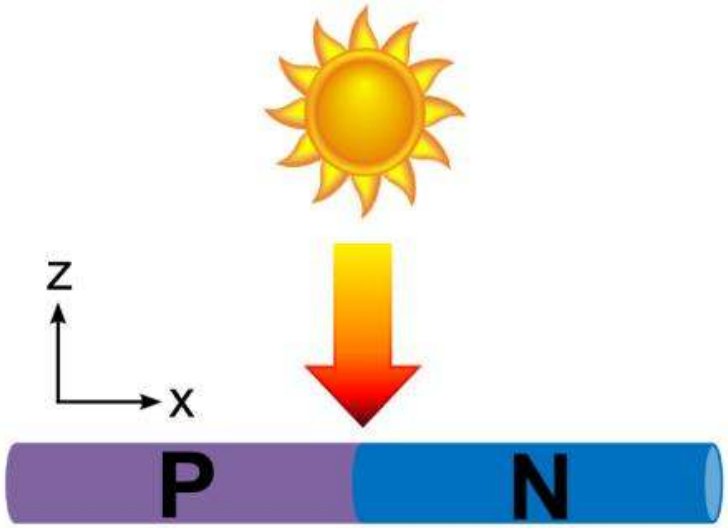
Electrons can absorb a photon leaving the device with higher energy

2 Si nanowire pn-junctions as photovoltaic device



SiNWs, [110] direction, 25 nm

NW-A 6656 atoms; NW-B 12672 atoms



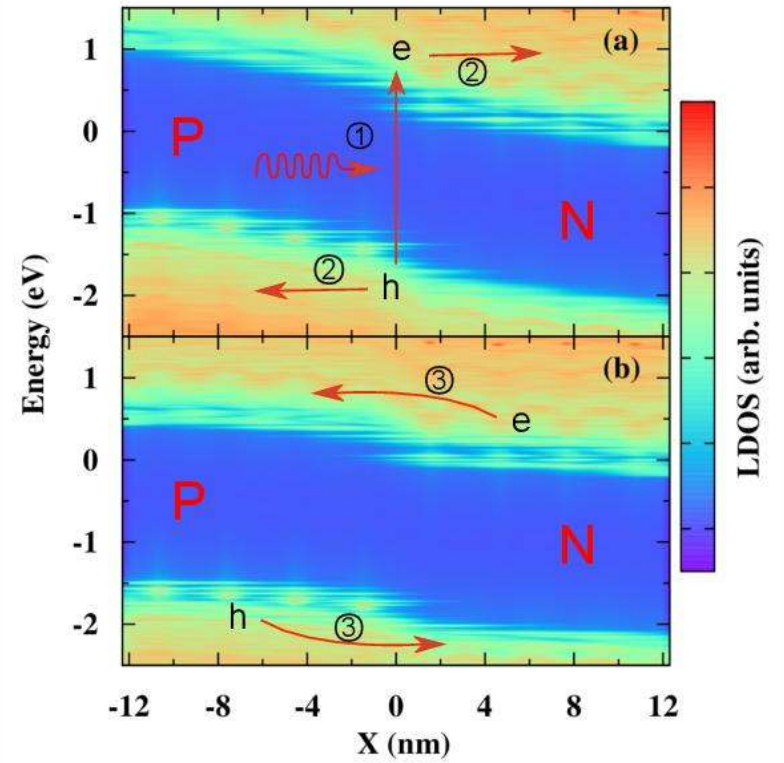
	Cross-section	Length	Doping concentration
NW-A	2nm x 2nm	25nm	8.0×10^{19} cm^{-3}
NW-B	3nm x 3nm	25nm	3.56×10^{19} cm^{-3}

I-V characteristics, short circuit current, open circuit voltage, power conversion efficiency

BCCMS

Zhang *et al*. JPC Lett. **5** (2014) 12

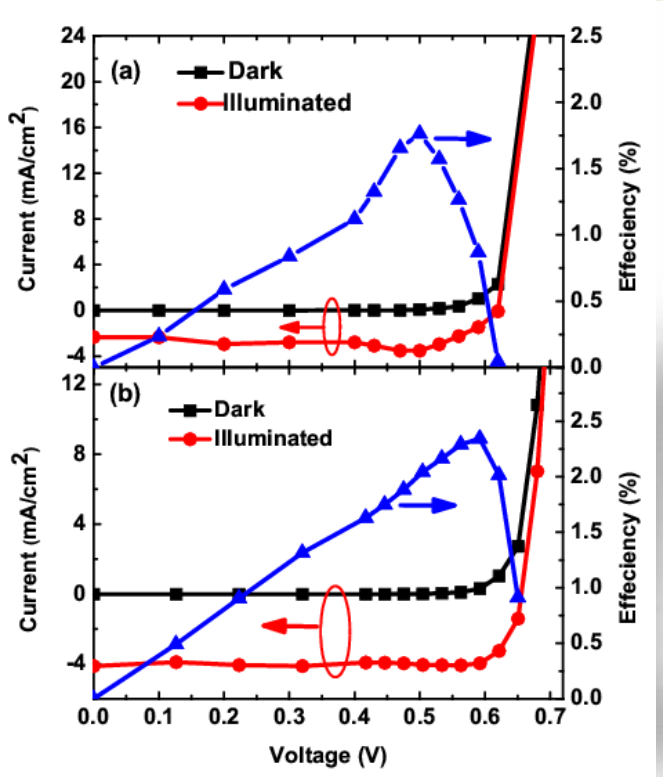
Simulation of photovoltaic device



LDOS of the NW-A with forward bias a) 0V b) 0.6V

Ban
volta

	NW-A	NW-B
I_{SC}	2.33 mA/cm^2	4.19 mA/cm^2
V_{OC}	0.62 V	0.66 V
α*	6.5%	12.4%

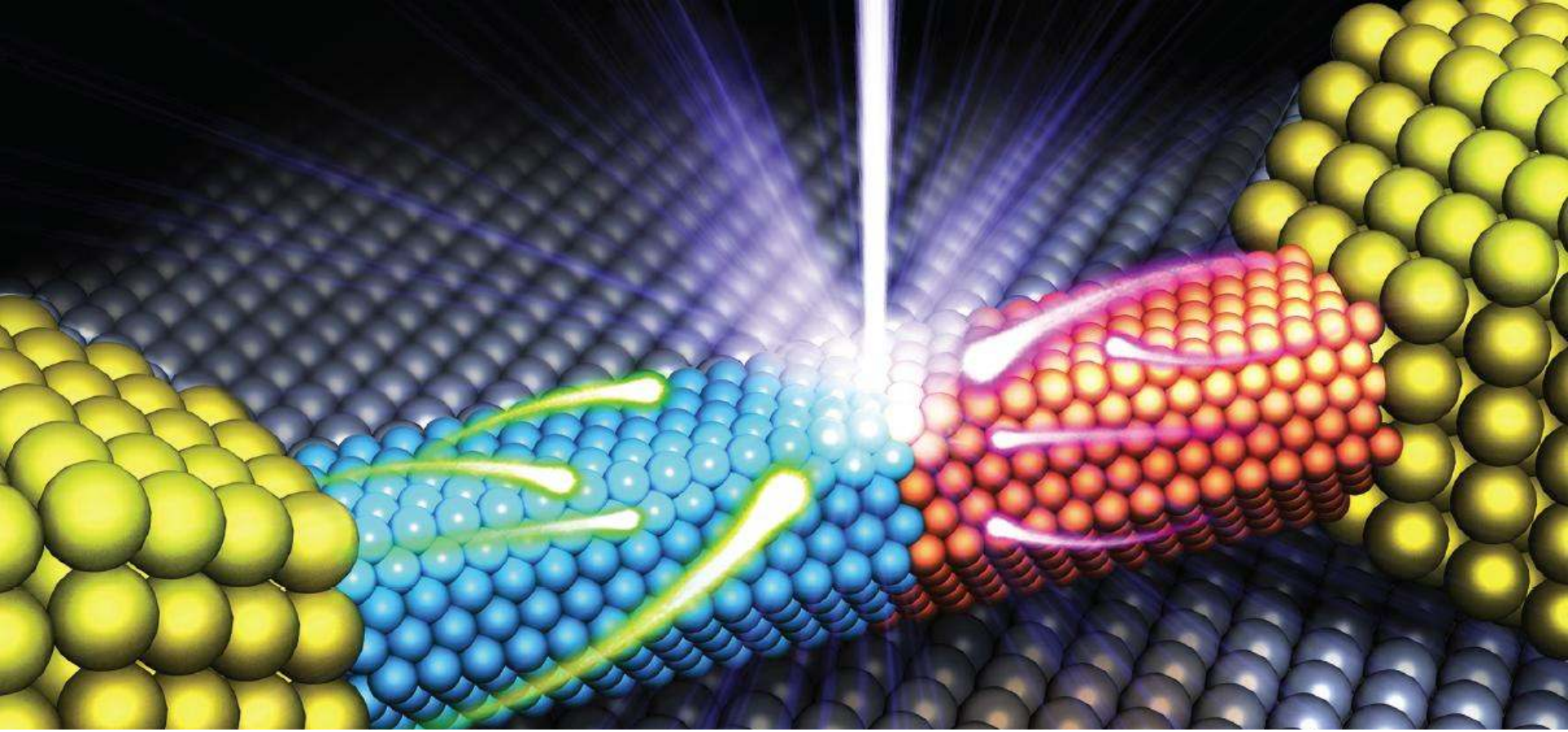


I-V curves of (a) NW-A and (b) NW-B with and without light illumination.

Photon energy is 2,5 eV

Enhancement by antireflection and light-trapping techniques

Zhang *et al*. JPC Lett. **5** (2014) 12



COMMUNICATION

ROYAL SOCIETY OF CHEMISTRY

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DOI: 10.1039/c6nr02356h

www.rsc.org/nanoscale

Quantum mechanical modeling the emission pattern and polarization of nanoscale light emitting diodes

Rulin Wang,[a] Yu Zhang,[b] Fuzhen Bi,[a,c] Thomas Frauenheim,[d] GuanHua Chen[e] and ChiYung Yam*[a,e]

Outline of the Talk

1. Brief introduction of the DFTB-method
2. Examples for device modeling
3. Ways to improve ground state accuracy and efficiency

4. TD-DFTB properties in linear response
5. NO-reduction on TiO_2 surfaces
6. Charge transfer exitations using pp-DFTB
7. Non-adiabatic Ehrenfest molecular dynamics

Improvement of ground and excited state accuracy

SCC-DFTB2 - consistent strong underestimation of Hydrogen bonds

Wrong qualitative description of Singlet-Triplet Excitations in TD-DFTB

Ways to improve ground state accuracy

- 3-rd order DFTB (DFTB3)
- Multipole interactions
- Onsite correction
- Many-body dispersion interactions (Tkatchenko et al. PRL 2012)

} highly improved H-bonds

All improvements are crucial for studies under environmental conditions, e.g. solvents and in particular for macromolecular systems

DFTB3

Qiang Cui (Madison) and Marcus Elstner

- Expansion of the total energy up to third order in $\delta n(\mathbf{r})$:

$$E_{\text{tot}} = E_{\text{bs}}[n_0] + E_{\text{rep}}[n_0] + E_2[n_0, \delta n^2] + E_3[n_0, \delta n^3]$$

$$E_3 = \frac{1}{3}\sum_A \sum_B q_A^2 q_B \Gamma_{AB}$$

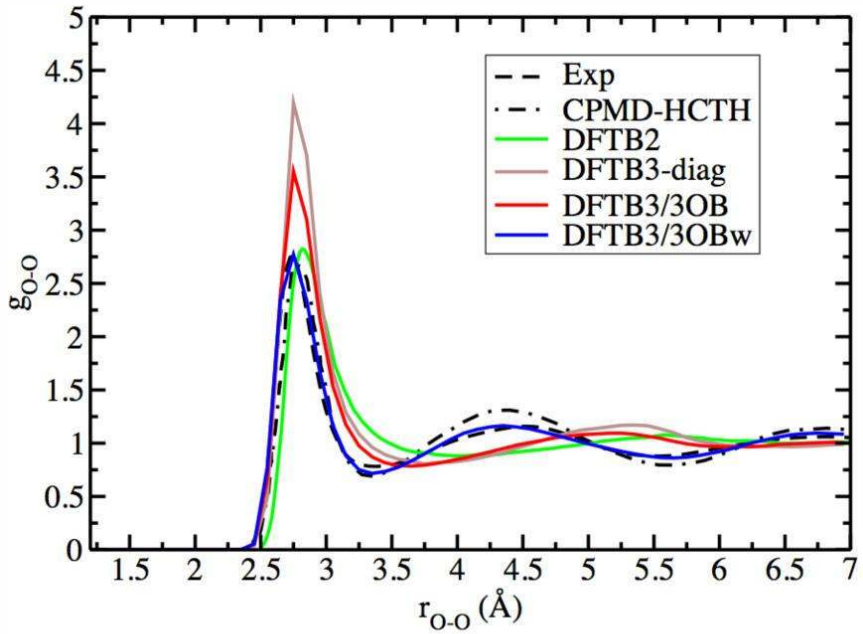
$$\Gamma_{AB} = \left.\frac{\partial \gamma_{AB}}{\partial U_A}\frac{\partial U_A}{\partial q_A}\right|_{q_A^0} \qquad \Gamma_{AA} = \left.\frac{1}{2}\frac{\partial \gamma_{AA}}{\partial U_A}\frac{\partial U_A}{\partial q_A}\right|_{q_A^0}$$

- Damping of γ_{AB} for hydrogen interactions:

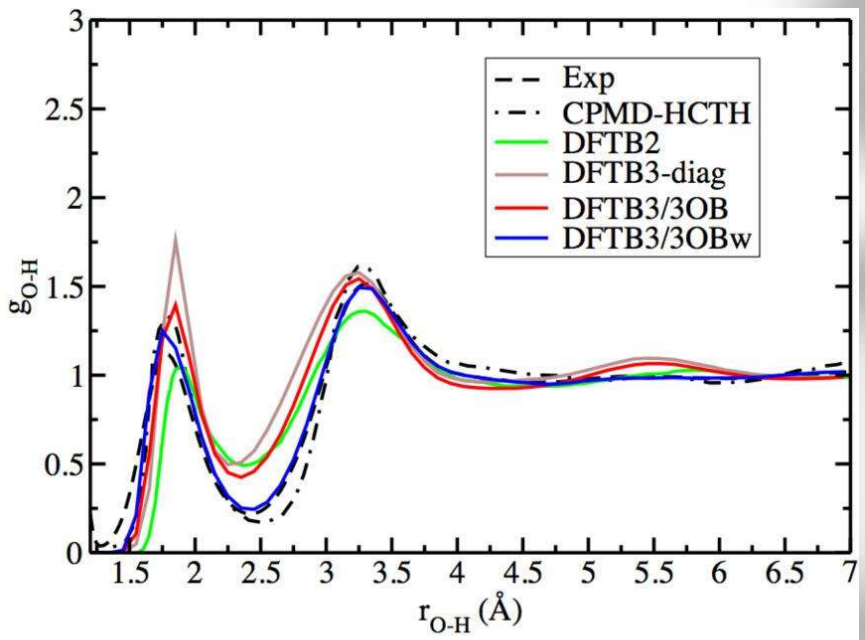
$$\tilde{\gamma}_{AB} = \frac{1}{R_{AB}} - s(R_{AB}, U_A, U_B)e^{-\left(\frac{U_A+U_B}{2}\right)^{\zeta} R_{AB}^2}$$

J. Chem. Theory Comput. 2013, 9, 338−354

DFTB3-QM/MM correct performance for treating water in different chemical environments



(a) g_{O-O}



(b) g_{O-H}

Minor changes in DFTB3 substantially improve the structural properties of bulk water under ambient conditions

JCTC Journal of Chemical Theory and Computation

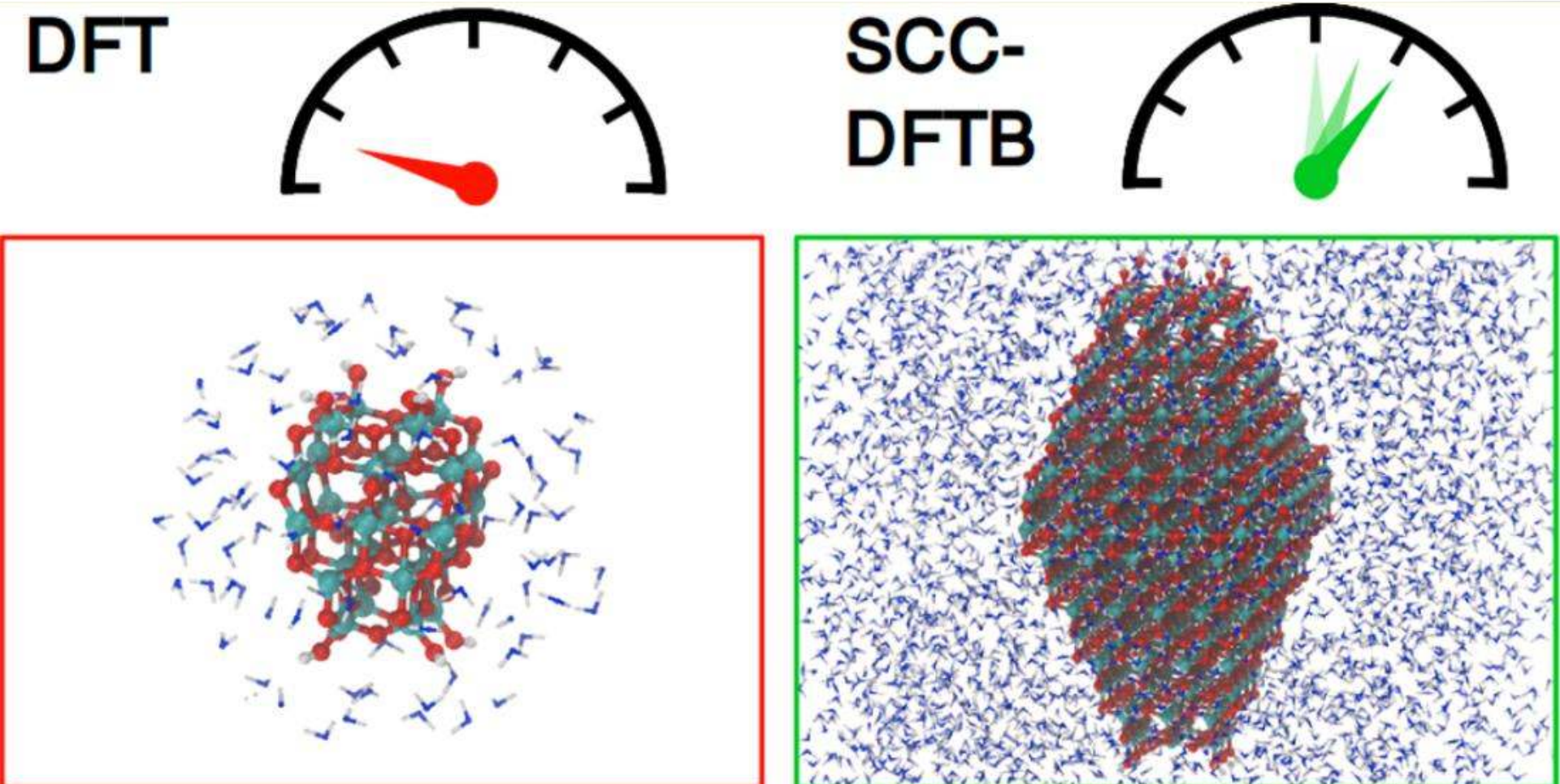
Article

pubs.acs.org/JCTC

DOI: 10.1021/acs.jctc.7b00479
J. Chem. Theory Comput. 2017, 13, 3862−3873

Water Multilayers on TiO_2 (101) Anatase Surface: Assessment of a DFTB-Based Method

Daniele Selli,[†] Gianluca Fazio,[†,‡] Gotthard Seifert,[‡] and Cristiana Di Valentin*[,†]



Many-body dispersion interaction for DFTB

THE JOURNAL OF CHEMICAL PHYSICS 144, 151101 (2016)

Communication: Charge-population based dispersion interactions for molecules and materials

Martin Stöhr,[1,2] Georg S. Michelitsch,[2] John C. Tully,[1] Karsten Reuter,[2] and Reinhard J. Maurer[1,a)]
[1]*Department of Chemistry, Yale University, New Haven, Connecticut 06520, USA*
[2]*Department Chemie, Technische Universität München, Lichtenbergstr. 4, D-85748 Garching, Germany*

(Received 3 March 2016; accepted 8 April 2016; published online 19 April 2016)

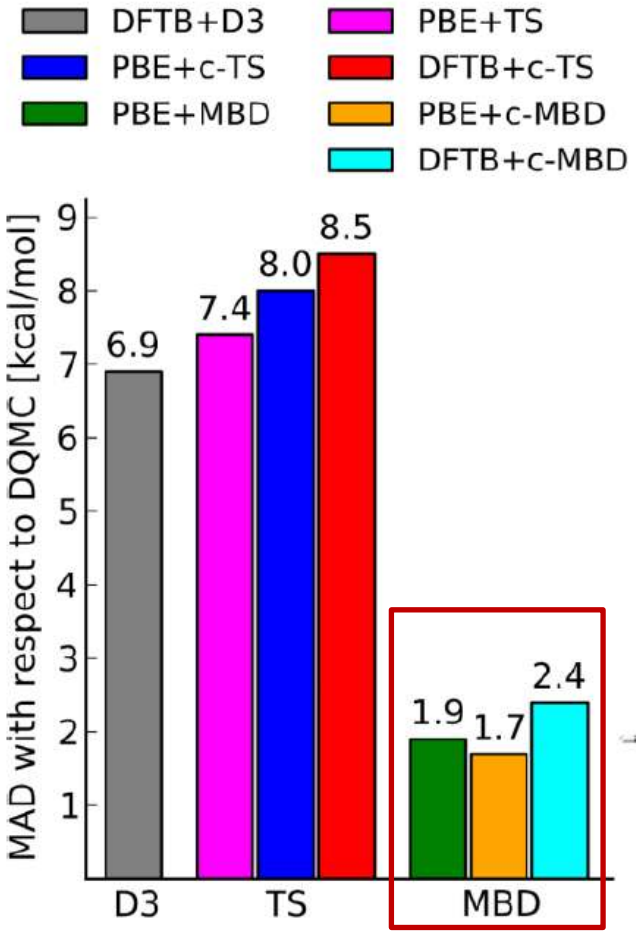
The DFT+vdW(TS), or in short DFT+TS, scheme[2] represents a particularly simple and accurate method to derive dispersion interactions directly from the electron density. The dispersion interaction as given by Eq. (1) is defined via effective atom-wise dispersion parameters such as static atomic polarizabilities α_A^0, C_6^{AA} coefficients, and van der Waals radii R_A

$$E_{\text{disp}} = -\sum_{A<B} f_{\text{damp}}(R_{AB}, R_A, R_B)\,\frac{C_6^{AB}}{R_{AB}^6},$$

$$C_6^{AB} = \frac{2\,C_6^{AA}C_6^{BB}}{\frac{\alpha_B^0}{\alpha_A^0}C_6^{AA} + \frac{\alpha_A^0}{\alpha_B^0}C_6^{BB}}. \qquad (2)$$

Tkatchenko et al. , Phys. Rev. Lett. 108 , 236402 (2012)

Many-body dipersion method for DFTB



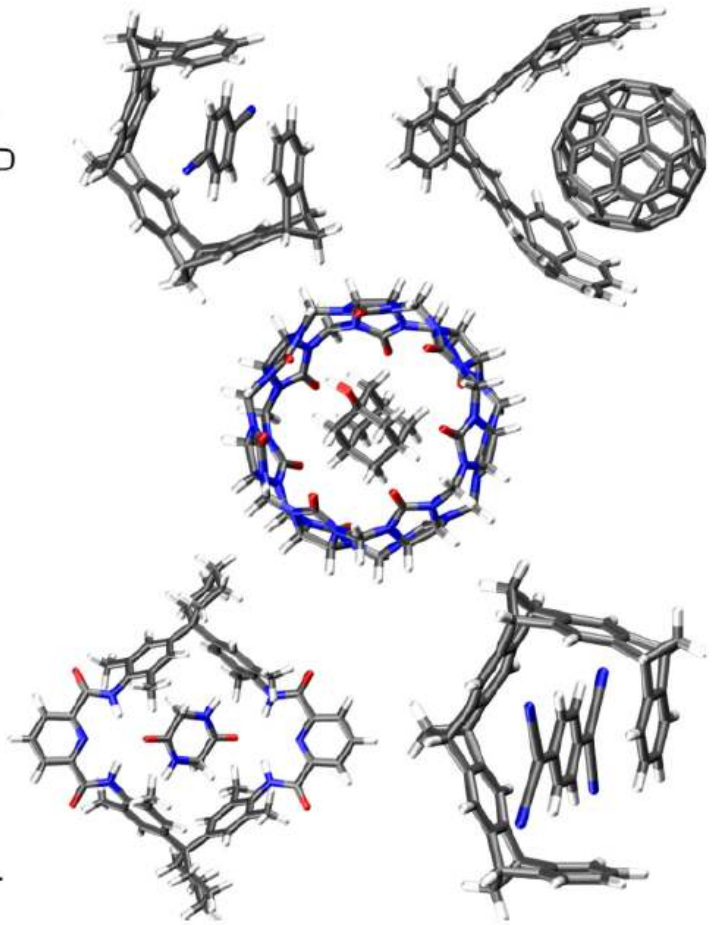


FIG. 2. Left: MADs in binding energies (in kcal/mol) for a selected subset of S12L complexes as obtained by different dispersion corrected approaches with respect to DQMC calculations. right: Graphical depiction of the S12L subset considered in this work. H (white), C (black), N (blue), O (red).

highly improved dispersion interactions

molecular crystals & supramolecular complexes

Molecular and organic electronics

Extended Lagrangian Born-Oppenheimer MD: XLBOMD

A. Niklasson

A. M. N. Niklasson, J. Chem. Phys. 130, 214109 (2009)
A. M. N. Niklasson and M. J. Cawkell, Phys. Rev. B 86, 174308 (2012)
http://www.dftb-plus.info

MD propagation without SCF cycles → speedup 1 orders of magnitude

DFTB-XLBOMD speedup 3 orders speedup versus conventional DFTB-BO-MD

In progress for release in 2018

- density matrix via a recursive expansion of the Fermi operator
- series of generalized sparse matrix algorithms
- Linear scaling matrix inversion
- efficient parallelisation using graph-based theory

C. Negre

DFTB+ 3 more orders speedup

- **1 time step 10^4 atoms in 0.1 sec**
- **100 ps QM-MD for 10^6 atoms**
- **Micro-second MD-simulations 10^4 atoms**
- **……..**

B. Aradi

BCCMS

Outline of the Talk

1. Brief introduction of the DFTB-method
2. Examples for device modeling
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4. **TD-DFTB properties in linear response**
5. **NO-reduction on TiO_2 surfaces**
6. **Charge transfer exitations using pp-DFTB**
7. **Non-adiabatic Ehrenfest molecular dynamics**

Review paper

Journal of Molecular Structure: THEOCHEM 914 (2009) 38–49

Contents lists available at ScienceDirect

Journal of Molecular Structure: THEOCHEM

journal homepage: www.elsevier.com/locate/theochem

Approximate time-dependent density functional theory

T.A. Niehaus *

Bremen Center for Computational Materials Science, Am Fallturm 1a, 28359 Bremen, Germany

Linear response treatment in the frequency domain

direct propagation in the time domain - Ehrenfest MD

and an O(N) implementation in the density matrix formalism

In linear response TD-DFT

Casida's equation

$$\Omega \mathbf{F}_I = \omega_I^2 \mathbf{F}_I$$

$$\sum_{jb} \left[\omega_{ia}^2 \delta_{ij} \delta_{ab} + 4\sqrt{\omega_{ia}} K^{\Sigma}_{ia,jb} \sqrt{\omega_{jb}} \right] F^{I\Sigma}_{jb} = \Omega^2_{I\Sigma} F^{I\Sigma}_{ia}$$

ω_I — excitation energies

$\mathbf{F}_I$ — excitation vectors

$$K^S_{ia,jb} = \int\int' \psi_i(\mathbf{r})\psi_a(\mathbf{r}) \left(\frac{1}{|\mathbf{r}-\mathbf{r}'|} + f_{xc}[\rho](\mathbf{r},\mathbf{r}') \right) \psi_j(\mathbf{r}')\psi_b(\mathbf{r}')$$

$$K^T_{ia,jb} = \int\int' \psi_i(\mathbf{r})\psi_a(\mathbf{r}) \left(\frac{\delta^2 E_{xc}}{\delta m(\mathbf{r})\, \delta m(\mathbf{r}')} \right) \psi_j(\mathbf{r}')\psi_b(\mathbf{r}')$$

TD-DFT: coupling matrix shifts the excitation energies

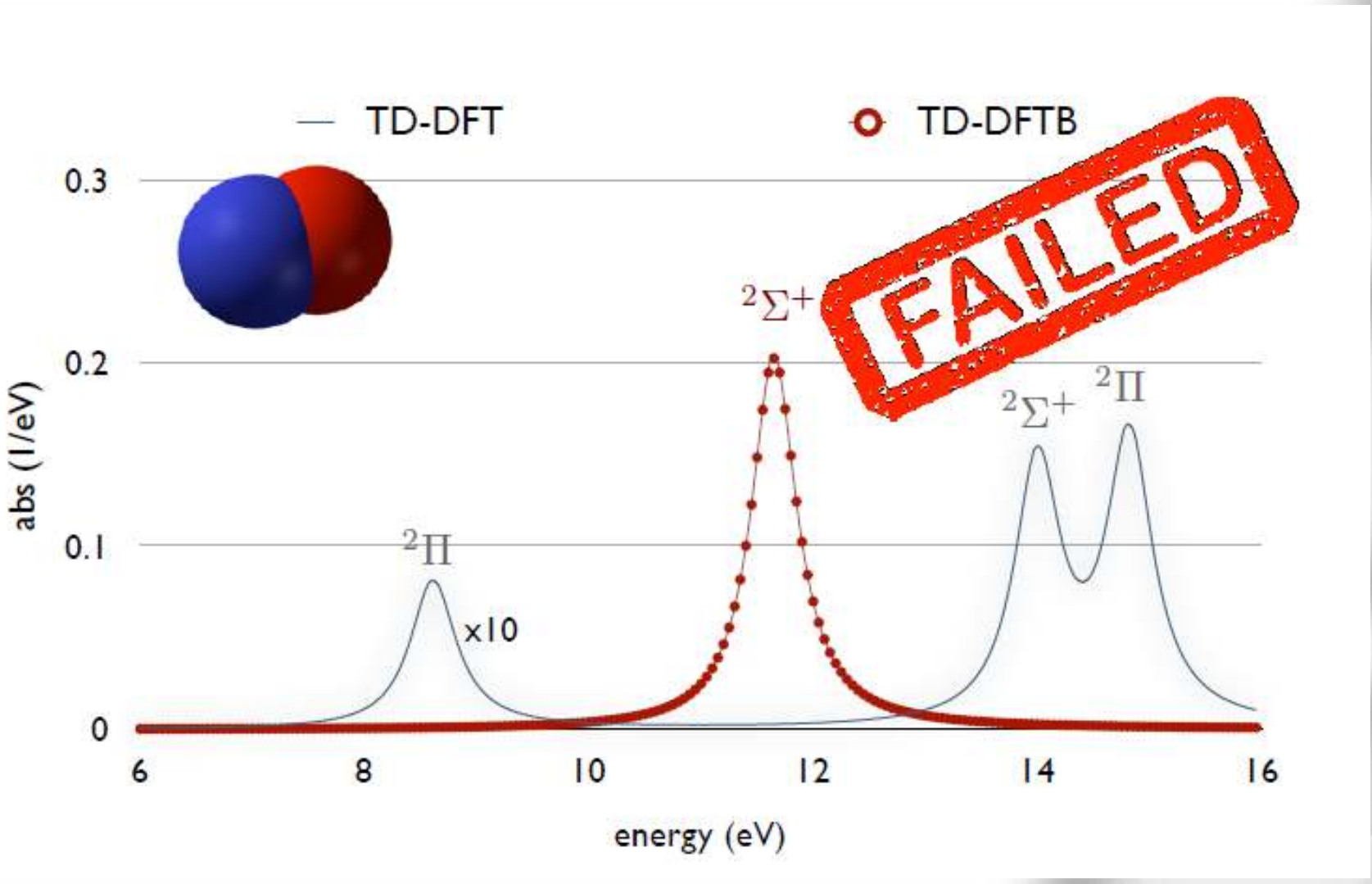
$$K^{DFTB}_{ia\sigma} = \sum_{ABll'} q^{ia\sigma}_{Al} \Gamma^{\sigma\tau}_{Al,Bl'} q^{jb\tau}_{Bl'}$$

Mulliken trans. charges

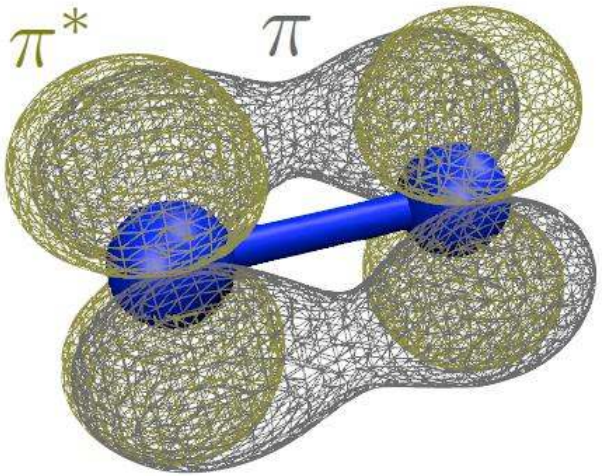
Mulliken approximation for transition dipole

$$\mathbf{d}_{ia\sigma} \approx \sum_{A} q^{ia\sigma}_{A} \mathbf{R}_A$$

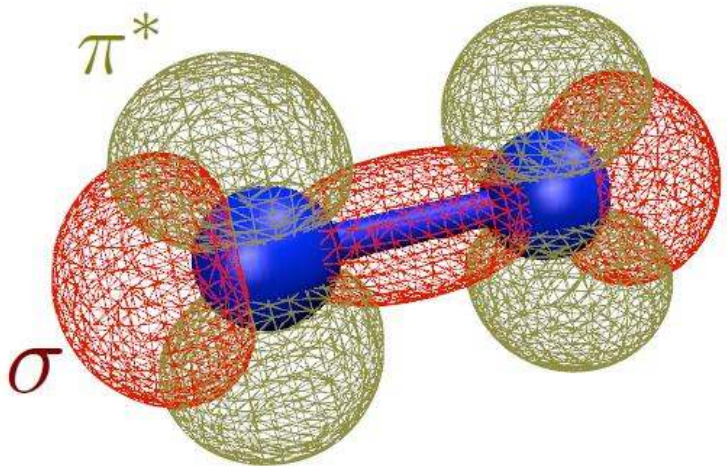
Absorption spectrum of NO with TD-DFTB without corrections



TD-DFTB excitations in the Mulliken approach



$\pi \rightarrow \pi^*$



$\sigma \rightarrow \pi^*$

$$\pi = c_{p_{1x}\pi} p_x^{(1)} + c_{p_{2x}\pi} p_x^{(2)}$$
$$\pi^* = c_{p_{1x}\pi^*} p_x^{(1)} - c_{p_{2x}\pi^*} p_x^{(2)}$$

$$q_1^{\pi\pi^*} = \frac{1}{2}(c_{p_{1x}\pi} c_{p_{1x}\pi^*} S_{p_{1x}p_{1x}} - c_{p_{1x}\pi} c_{p_{2x}\pi^*} S_{p_{1x}p_{2x}})$$

$$\sigma = c_{p_{1z}\pi} p_z^{(1)} + c_{p_{2z}\pi} p_z^{(2)}$$
$$\pi^* = c_{p_{1x}\pi^*} p_x^{(1)} - c_{p_{2x}\pi^*} p_x^{(2)}$$

$$q_1^{\sigma\pi^*} = \frac{1}{2}(c_{p_{1z}\sigma} c_{p_{1x}\pi^*} \overset{0}{S_{p_{1z}p_{1x}}} - c_{p_{1z}\pi} c_{p_{2x}\pi^*} \overset{0}{S_{p_{1z}p_{2x}}})$$

$$\omega_I = \omega_{\sigma\pi^*} \qquad \mathrm{d}_{\sigma\pi^*} = 0$$

Correct coupling

Transition charges are zero – no coupling even dipole-forbidden

JCTC Journal of Chemical Theory and Computation

Article

pubs.acs.org/JCTC

9 (2013) 4901

Extensions of the Time-Dependent Density Functional Based Tight-Binding Approach

A. Domínguez,*[,†] B. Aradi,[†] T. Frauenheim,[†] V. Lutsker,[‡] and T. A. Niehaus[‡]

[†]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1, 28359 Bremen, Germany

[‡]Department of Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Supporting Information

ABSTRACT: The time-dependent density functional based tight-binding (TD-DFTB) approach is generalized to account for fractional occupations. In addition, an on-site correction leads to marked qualitative and quantitative improvements over the original method. Especially, the known failure of TD-DFTB for the description of $\sigma \rightarrow \pi^*$ and $n \rightarrow \pi^*$ excitations is overcome. Benchmark calculations on a large set of organic molecules also indicate a better description of triplet states. The accuracy of the revised TD-DFTB method is found to be similar to first principles TD-DFT calculations at a highly reduced computational cost. As a side issue, we also discuss the generalization of the TD-DFTB method to spin-polarized systems. In contrast to an earlier study, we obtain a formalism that is fully consistent with the use of local exchange-correlation functionals in the ground state DFTB method.

Onsite correction: improved accuracy for excitation energies in TD-DFTB

- Mulliken-approximation for orbital products:

$$\phi_\mu(\mathbf{r})\phi_\nu(\mathbf{r}) \approx \frac{1}{2} S_{\mu\nu}(|\phi_\mu(\mathbf{r})|^2 + |\phi_\nu(\mathbf{r})|^2)$$

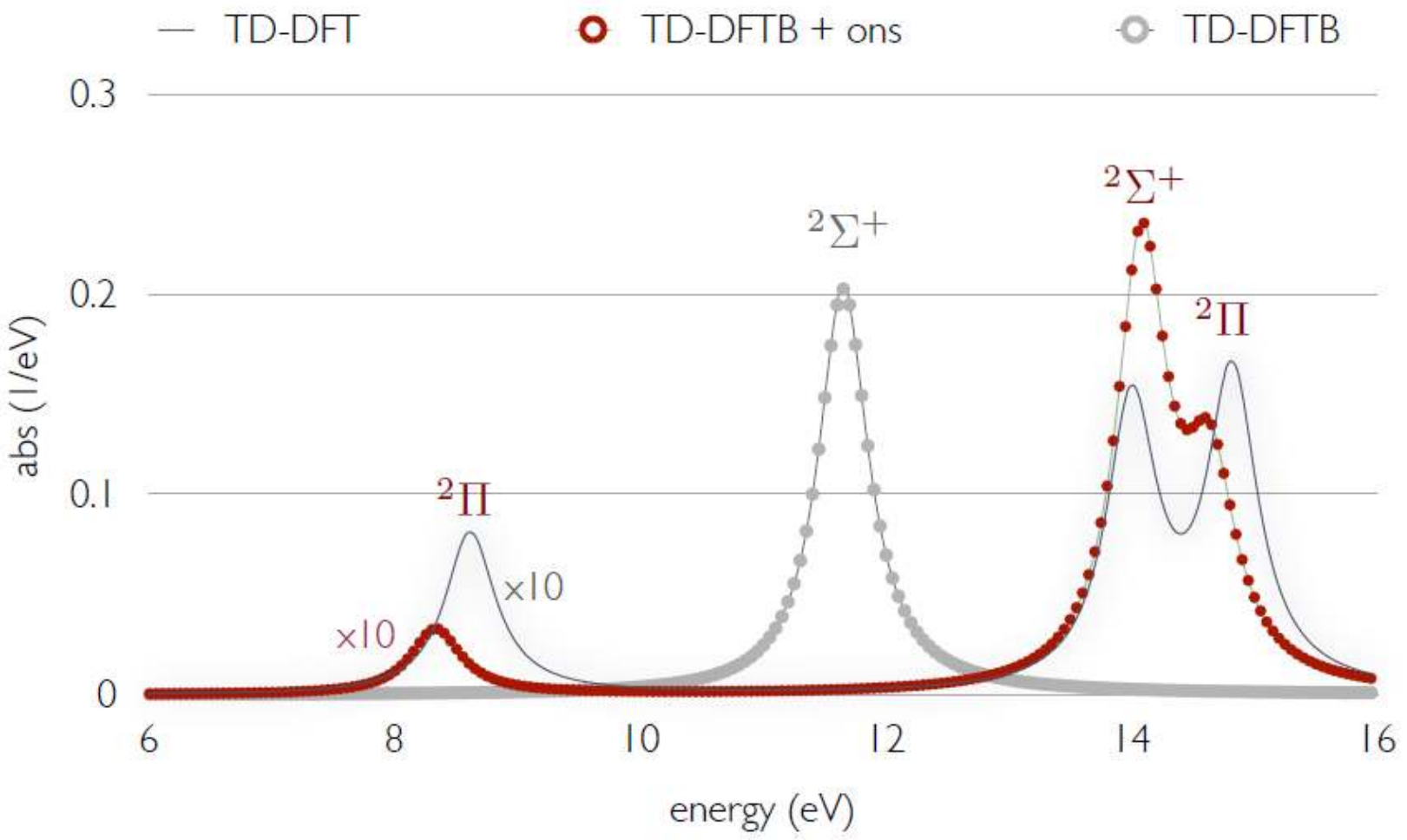
- Going beyond Mulliken-approximation:

$$E_2 = \frac{1}{2}\Big[\sum_{\mu\nu} \Delta\tilde{P}_{\mu\mu}(\mu\mu|\nu\nu)\Delta\tilde{P}_{\nu\nu} + \sum_{A}\sum_{\mu,\nu_A}^{\mu\neq\nu} \Delta\tilde{P}_{\mu\nu}(\mu\nu|\mu\nu)\Delta\tilde{P}_{\mu\nu} + \ldots\Big]$$

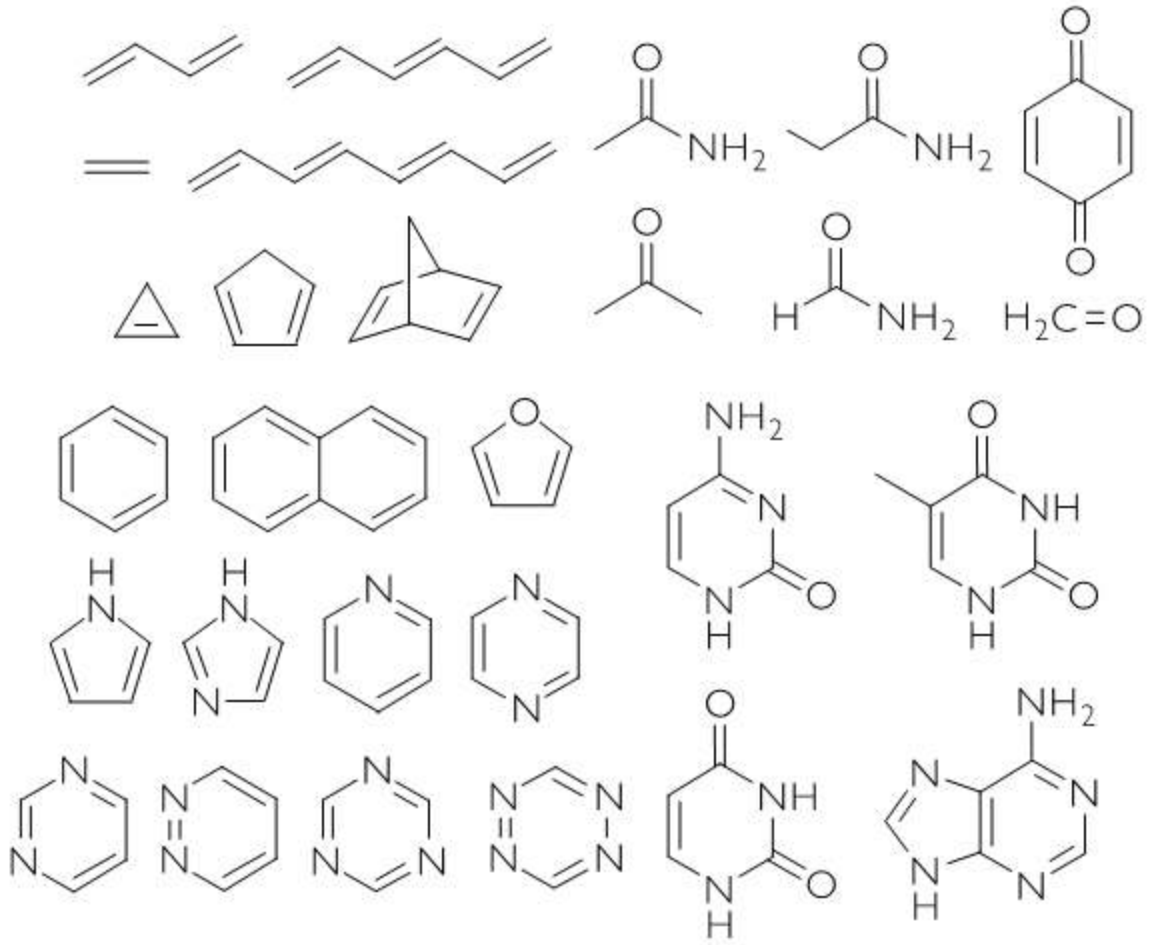
$$\Delta\tilde{P} = \Delta P\, S$$

A. Dominguez et. al, JCTC 9, 4901 (2013)

Absorption spectrum of NO with onsite corrections



Performance – Thiel´s benchmark set



28 compounds

TBE

104 singlet-triplet excitations

63 singlet-singlet excitations

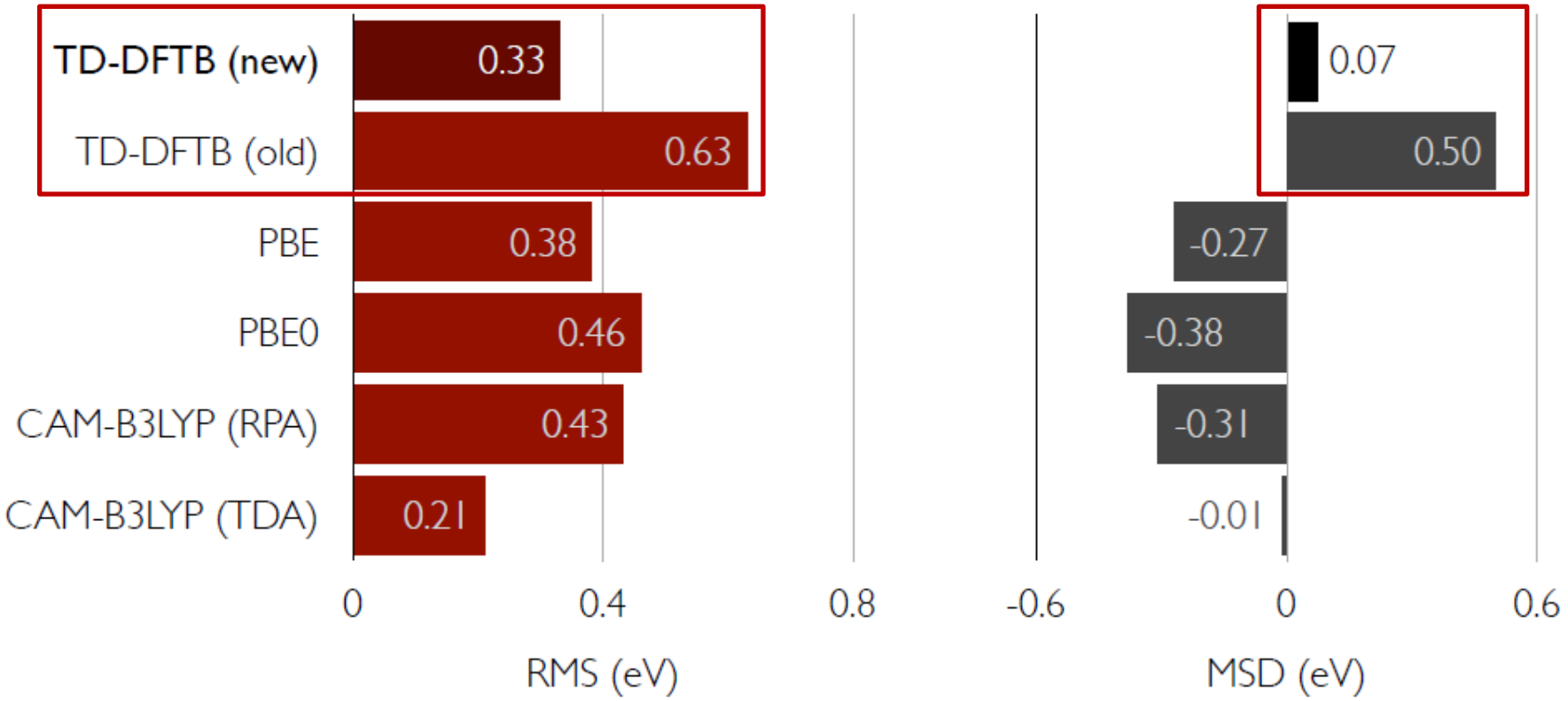
Experiment

80 singlet-triplet excitations

30 singlet-singlet excitations

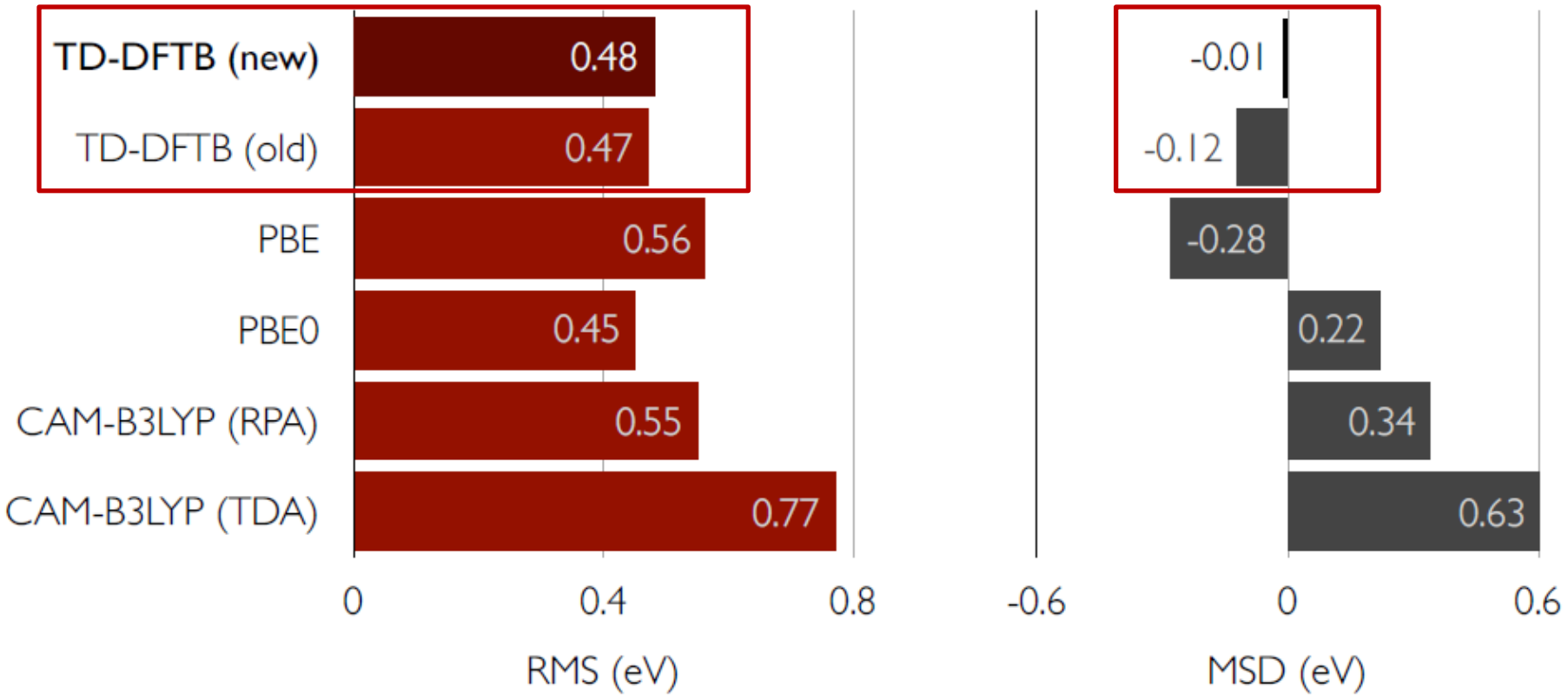
Singlet and triplet vertical excitations compared to TD-DFT PBE, PBE0, CAM-B3LYP

RMS error and MSD for singlet-triplet transition energies



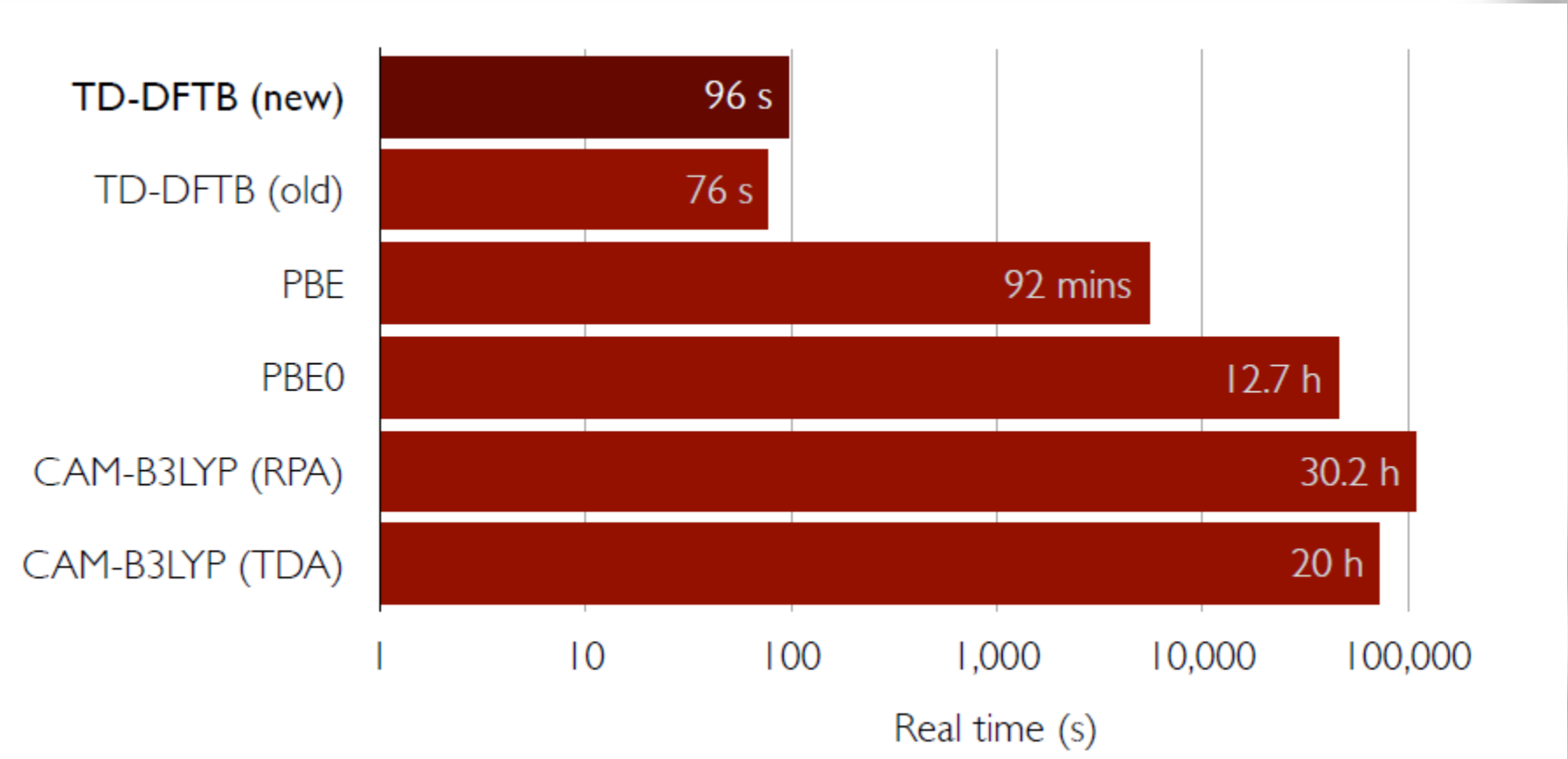
Thiel´s benchmark set compared to **experimental data**

RMS error and MSD for singlet-singlet transition energies



Thiel´s benchmark set compared to **experimental data**

Total wall clock time Thiel´s set singlet and triplets excitations



Thiel´s benchmark subset

THE JOURNAL OF PHYSICAL CHEMISTRY C

Article

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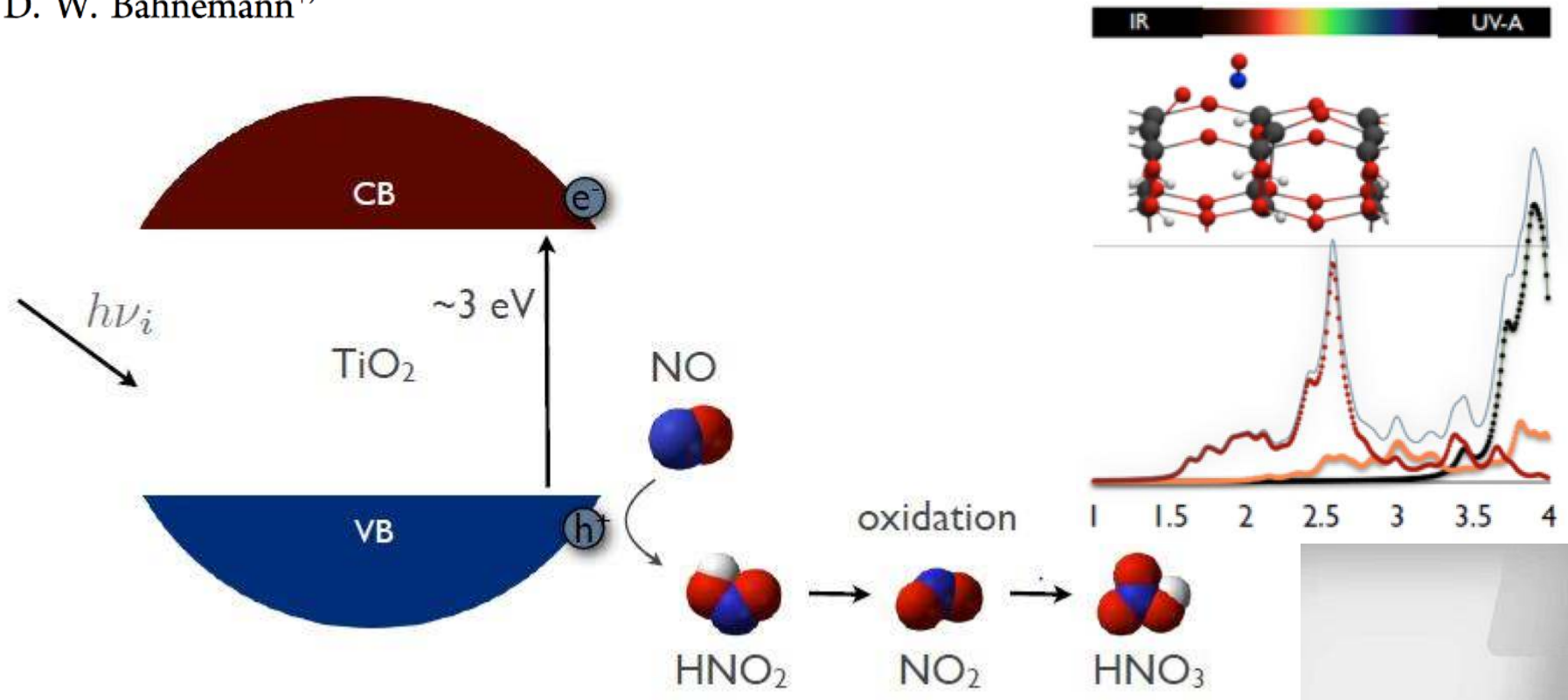
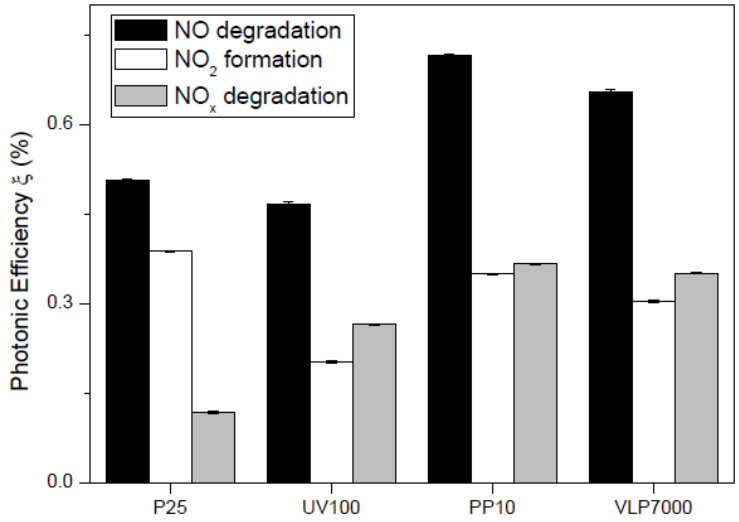
DOI: 10.1021/jp5108069
J. Phys. Chem. C 2015, 119, 4488−4501

Nitrogen(II) Oxide Charge Transfer Complexes on TiO_2: A New Source for Visible-Light Activity

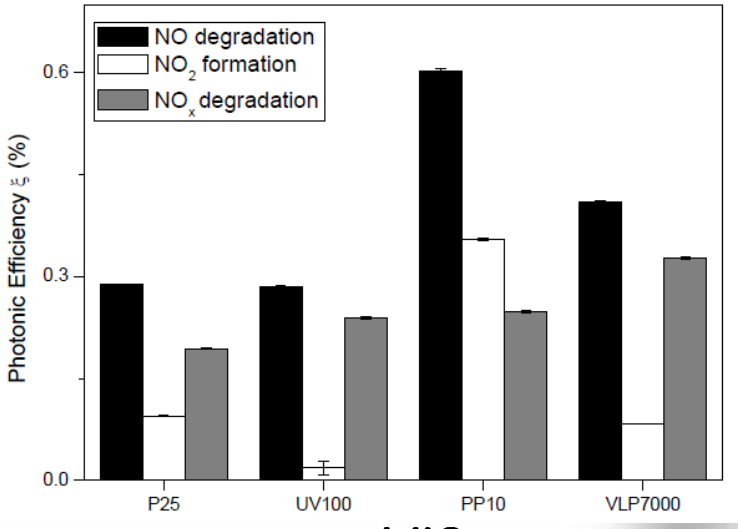
J. Freitag,[†] A. Domínguez,*[,‡] T. A. Niehaus,[¶] A. Hülsewig,[§] R. Dillert,[†] T. Frauenheim,[‡] and D. W. Bahnemann[†,⊥]



Photonic efficiencies of four TiO_2 powders under UV and VIS



UV



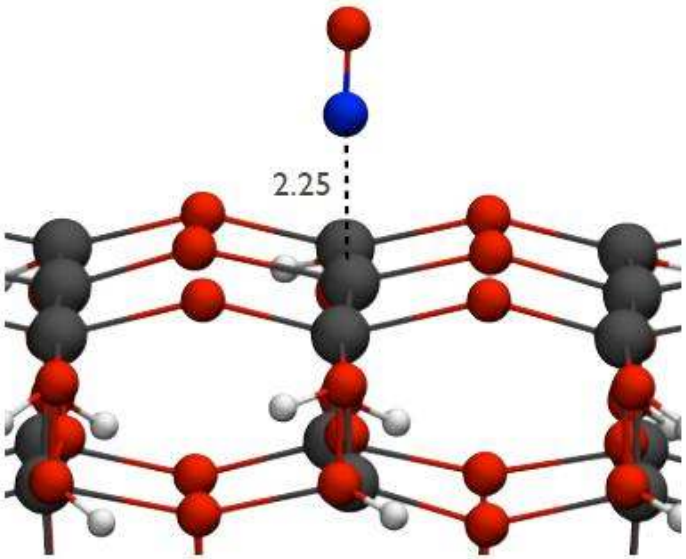
VIS

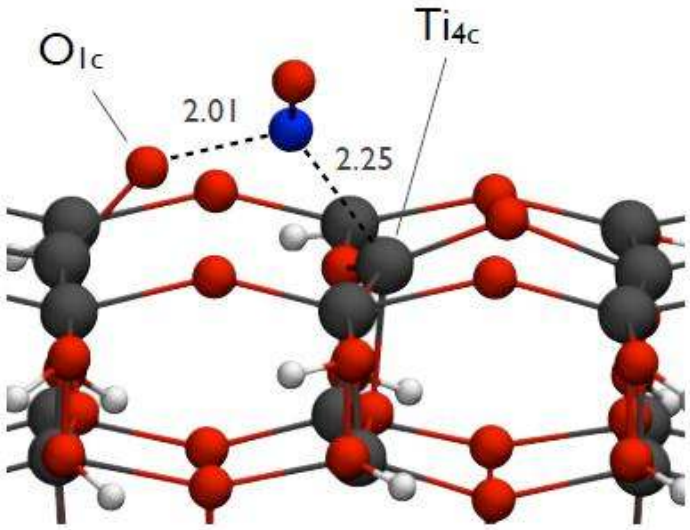
TiO_2 powder	Selectivity (UV) /%	Selectivity S (Visible) /%
P25	23.44	67.03
UV100	56.75	83.62
PP10	51.51	41.15
VLP 7000	53.51	79.77

Pollutant – TiO_2 hybrid complexes are photo-active in the visible light

Experiments Uni-Hannover – Detlef Bahnemann

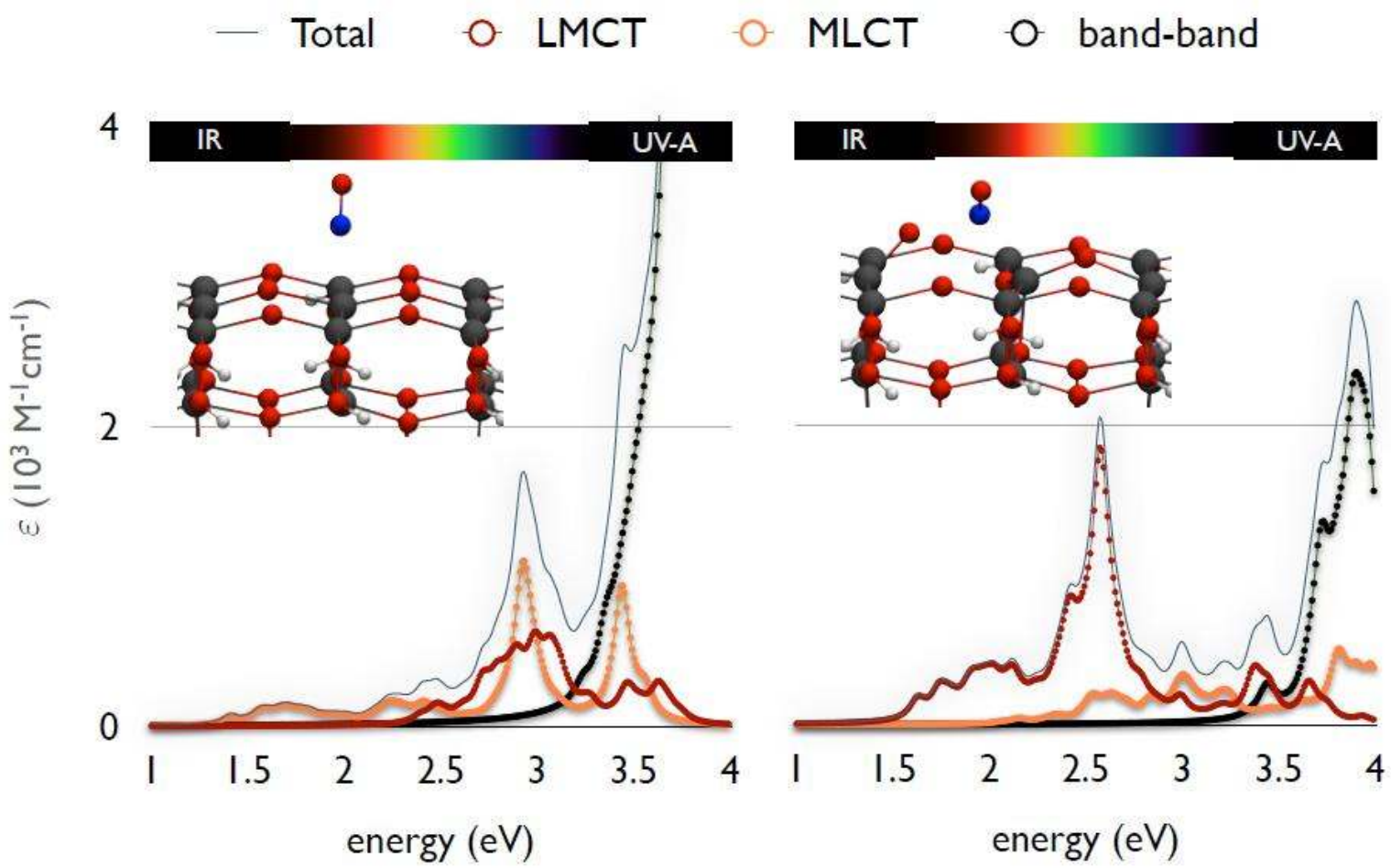
Two stable NO adsorption sites on anatase TiO_2





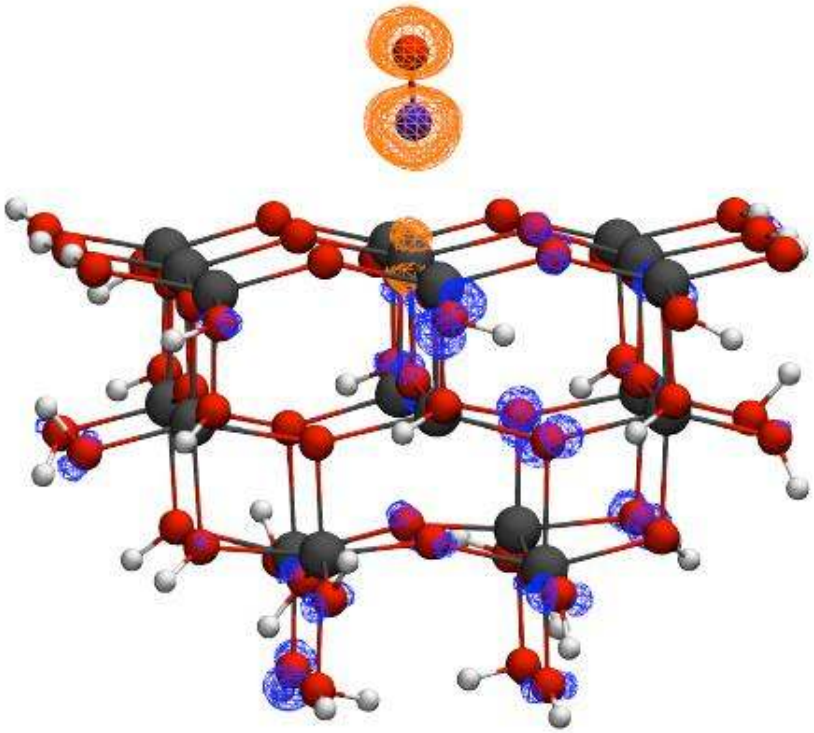
Scanning NO-adsorption for most stable sites on anatase (110)

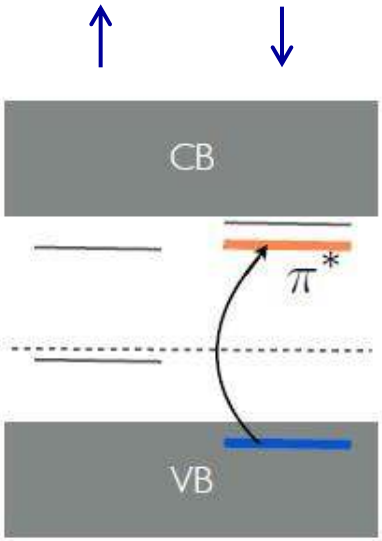
Two stable NO adsorption sites on anatase TiO_2

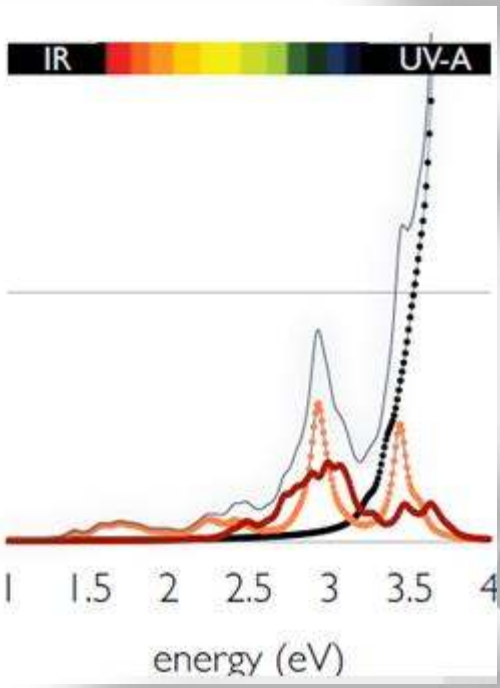


Strongly enhanced visible light activity

NO adsorption spectra on anatase TiO_2 (001) surface

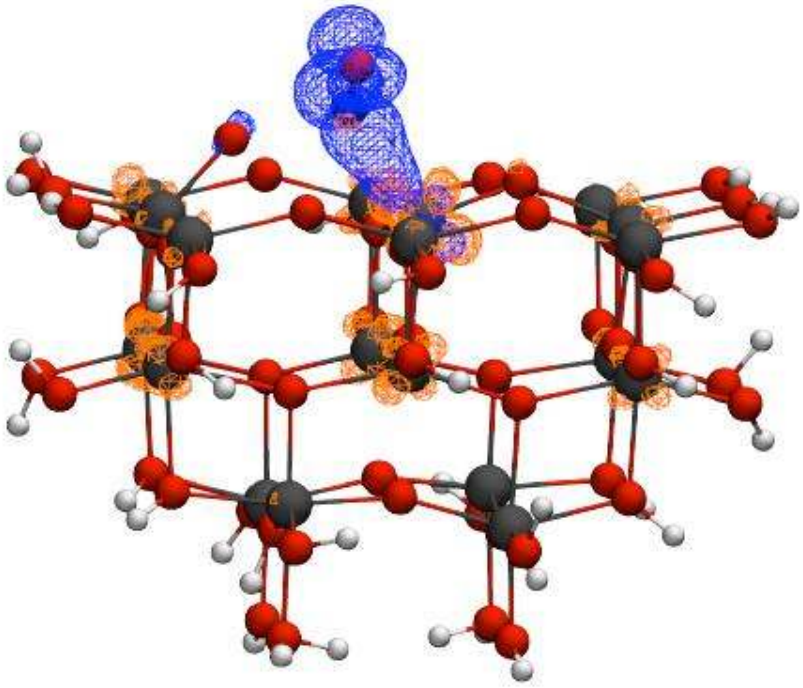


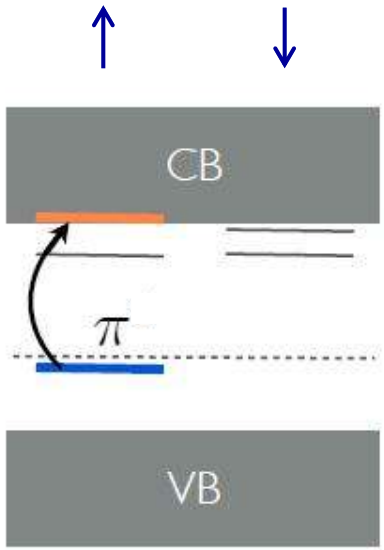


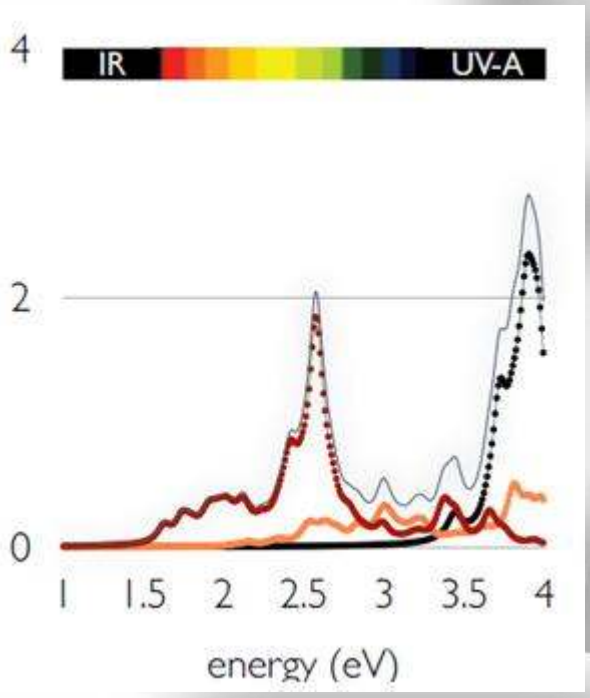


Charge transfer from TiO_2 valence band to NO-π* molecular orbital

NO adsorption spectra on anatase TiO_2 surface







Charge transfer from NO-π orbital to TiO_2 conduction band

Freitag, Dominguez, et al. J. Phys. Chem. C, ***119*** *(2015) 4488*

BCCMS

Outline of the Talk

1. Brief introduction of the DFTB-method
2. Examples for device modeling
3. Ways to improve ground state accuracy for H-bonds and dispersion

4. TD-DFTB properties in linear response
5. NO-reduction on TiO_2 surfaces
6. Charge transfer exitations using pp-DFTB
7. **Non-adiabatic molecular dynamics**

JCTC Journal of Chemical Theory and Computation

J. Chem. Theory Comput. 2016, 12, 1436−1448

Nonadiabatic Molecular Dynamics for Thousand Atom Systems: A Tight-Binding Approach toward PYXAID

Sougata Pal,[†] Dhara J. Trivedi,[‖] Alexey V. Akimov,[§] Bálint Aradi,[‡] Thomas Frauenheim,[‡] and Oleg V. Prezhdo*[,†]

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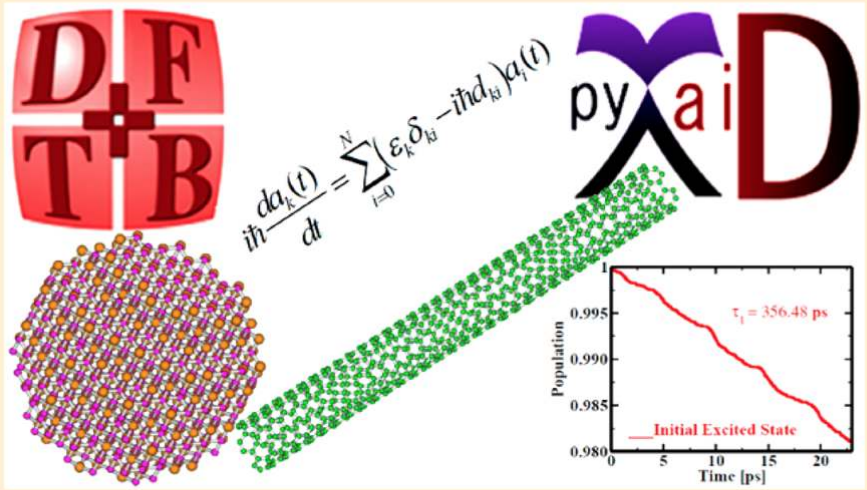
ABSTRACT: Excited state dynamics at the nanoscale requires treatment of systems involving hundreds and thousands of atoms. In the majority of cases, depending on the process under investigation, the electronic structure component of the calculation constitutes the computation bottleneck. We developed an efficient approach for simulating nonadiabatic molecular dynamics (NA-MD) of large systems in the framework of the self-consistent charge density functional

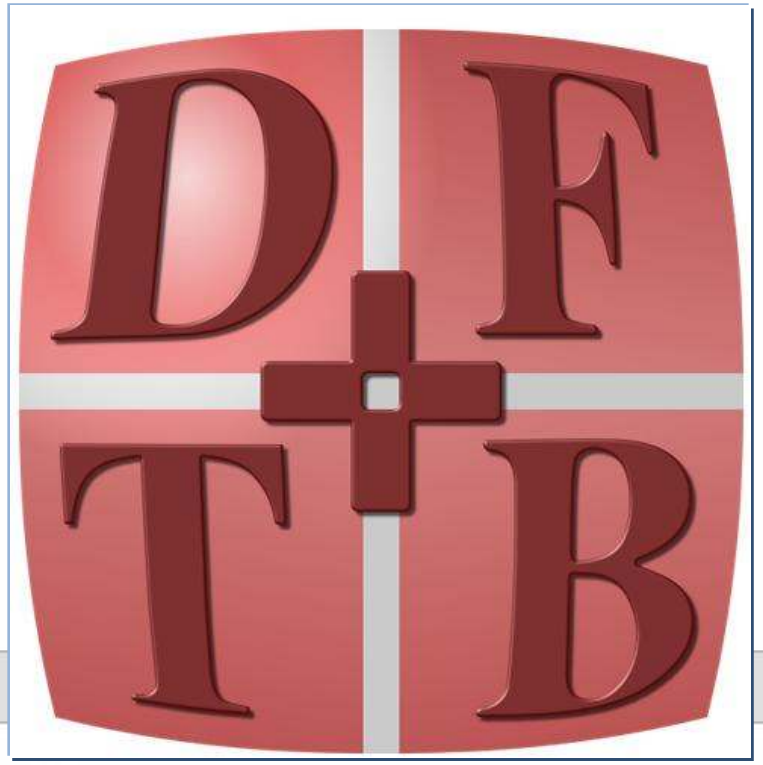
combined SH) and niques for e Python simulation esigned to veloped approach is tested with *ab initio* DFT and experimental data, by nd nonradiative electron−hole recombination in a CdSe quantum dot and nique is capable of treating accurately and efficiently excitation dynamics in t computational resources.



DFTB+ as electronic structure driving engine for NAMD in PYXAID

- Adiabatic electronic state energies
- NA couplings, d_{ki},
- Interatomic forces acting on the nuclei

as essential input quantities for NA-MD simulations



$$i\hbar \frac{dc_k(t)}{dt} = \sum_{i=0}^{N} (\varepsilon_k \delta_{ki} - i\hbar d_{ki}) c_i(t)$$

where

$$d_{ki} = \left\langle \phi_k(r, R(t)) \left| \frac{\partial \phi_i(r, R(t))}{\partial t} \right. \right\rangle$$

DFTB+ as driving engine for NAMD in NEXMD (Los Alamos)

- **NEXMD** with various surface hopping techniques
- Real-time NAMD
- Based on excited state determinants
- Available in combination with SE methods, like AM_x

Interface to AMBER force field: excited state QM/MM

Sergei Tretiak LANL

Adrian Roitberg U Florida

NEW implementation of real time TDDFTB: electron-ion dynamics

Christian Sanchez (right), Franco Bonafe, University of Cordoba

Numerical propagation of density matrix according to Liouville-von Neumann equation

$$\dot{\rho} = -i(S^{-1}H\rho - \rho H S^{-1}) \rightarrow \rho_{i+1} = \rho_{i-1} + 2\Delta t\dot{\rho}_i$$

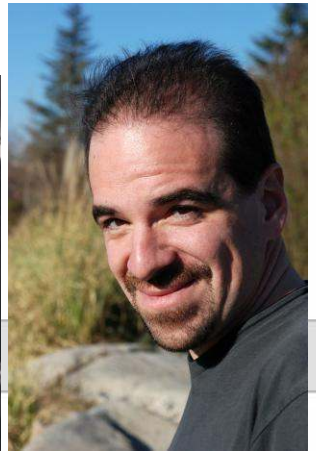
$$H_{\mu\nu} = H^0_{\mu\nu} + \frac{1}{2}S_{\mu\nu}\sum_K(\gamma_{IK} + \gamma_{JK})\Delta q_K, \quad \mu \in I \quad \nu \in J.$$

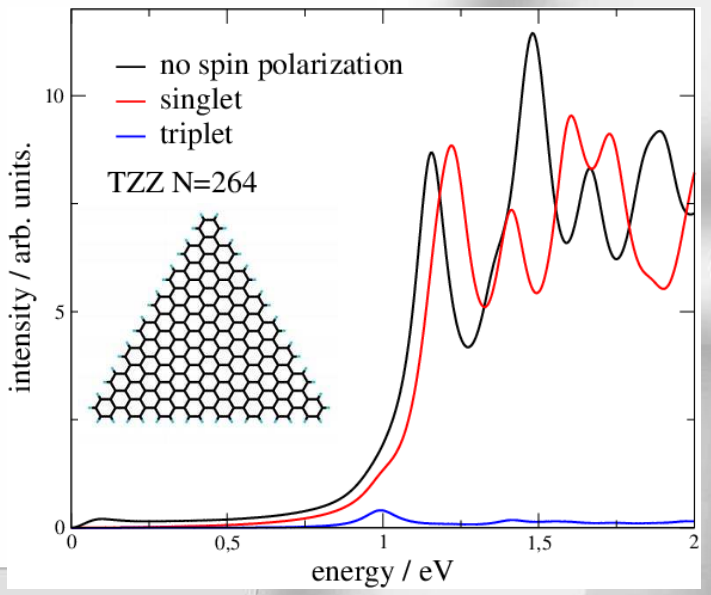
Absorption spectra are calculated by the polarizability tensor obtained by Fourier transform of the dipole moment, after a proper perturbation

$$\mu(t) = \int_{-\infty}^{\infty} \alpha(t-\tau)E(\tau)\mathbf{d}\tau$$

$$E(t) = E_0\delta(t - t_0)$$

Initial kick determines type of spectrum:
- Electric field: singlet spectrum
- Magnetic field: triplet spectrum

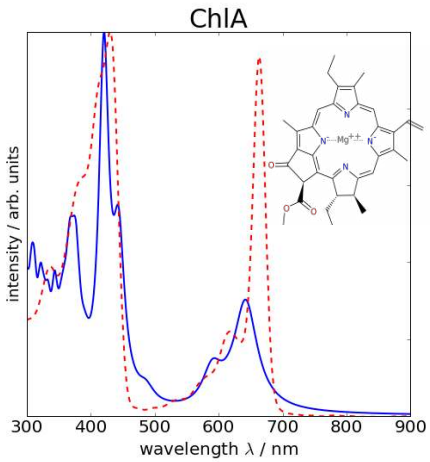


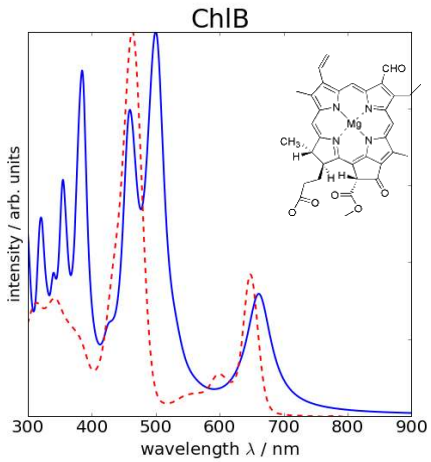


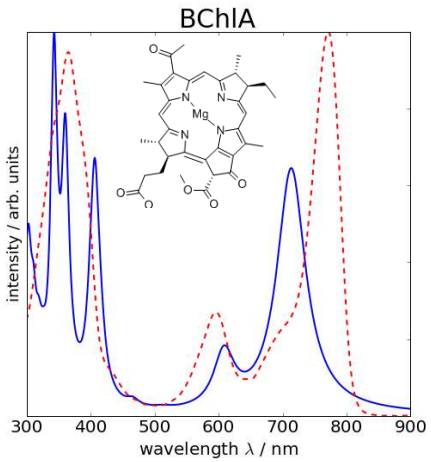
Zigzag graphene nanoflake

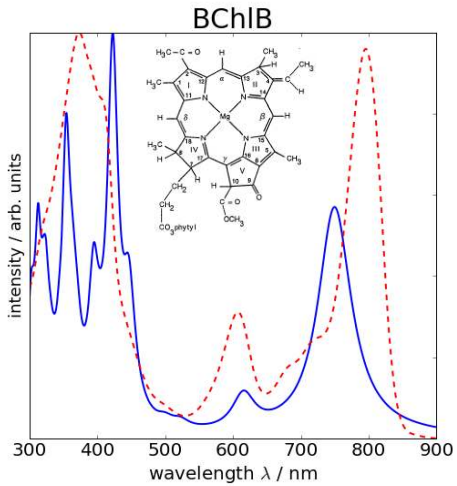
BCCMS

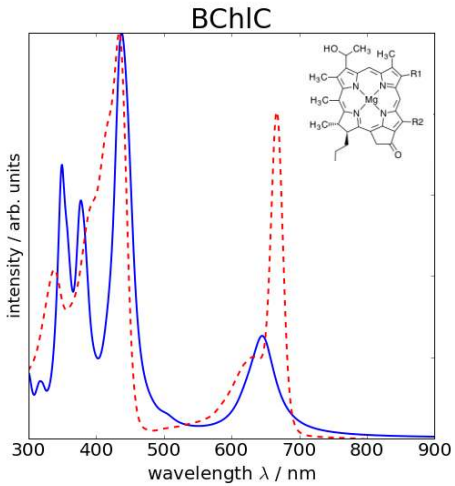
Absorption spectra of photosynthetic pigments

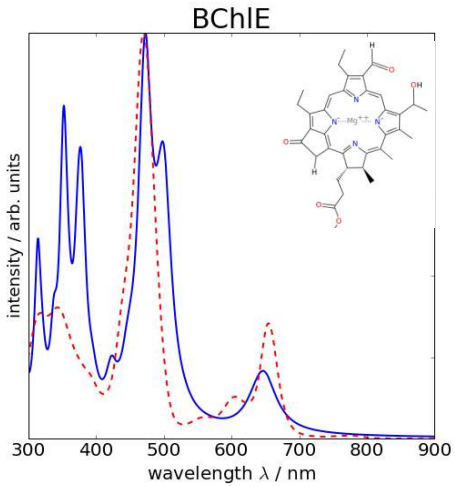












Experimental data in agreement with calculated frequencies and intensities

Experimental

Calculated with TDDFTB in DFTB+

Non-adiabatic Ehrenfest dynamics

Semi-classical treatment: **classical nuclei, quantum electrons.**

Equation of motion of density matrices includes
non-adiabatic coupling matrix and velocity dependent terms:

$$\dot{\rho} = -i(S^{-1}H\rho - \rho H S^{-1}) - (S^{-1}\tilde{D}\rho + \rho\tilde{D}S^{-1})$$

Ion dynamics by **velocity-Verlet**:

$$\mathbf{R}_A(t+\Delta t) = \mathbf{R}_A(t) + \dot{\mathbf{R}}_A(t)\Delta t + \tfrac{1}{2m}\mathbf{F}_A(t)\Delta t^2$$
$$\dot{\mathbf{R}}_A(t+\Delta t) = \dot{\mathbf{R}}(t) + \tfrac{1}{2m}(\mathbf{F}_A(t) + \mathbf{F}_A(t+\Delta t))\Delta t$$

$$\tilde{D}_{kl} = \dot{\mathbf{R}}_A \cdot \langle \phi_k | \nabla_A \phi_l \rangle$$

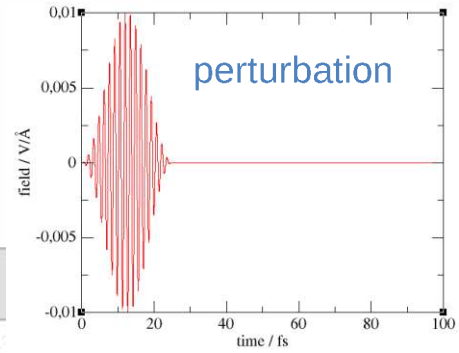
$v_A \cdot \nabla_A S_{kl}$ Todorov

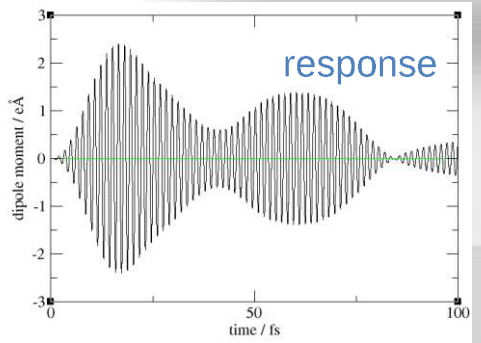
The electric field is added as any external perturbation to the hamiltonian:

$$H = H^1 + \tfrac{1}{2}(Sf + fS) \qquad \text{where} \qquad f = -e\mathbf{E}(t)\cdot\hat{\mathbf{r}}$$

For a $\sin^2$ laser pulse of length τ with frequency ω, e.g., the electric field is:

$$\mathbf{E}(t) = E_0 \sin^2(\pi t/\tau)\sin(\omega t)(1-\Theta(\tau))$$





Impulsive breathing mode excitations in Ag and Au NPs

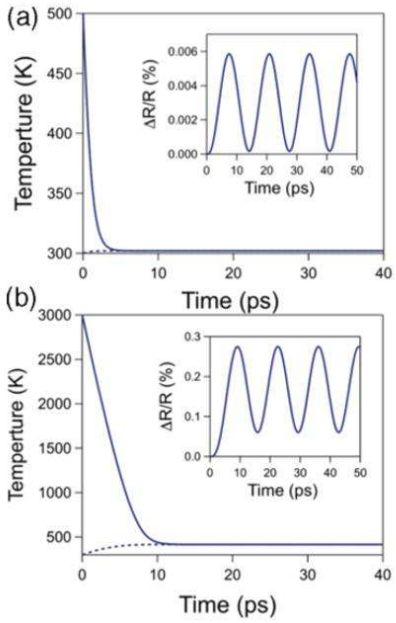
Motivation by experimental studies

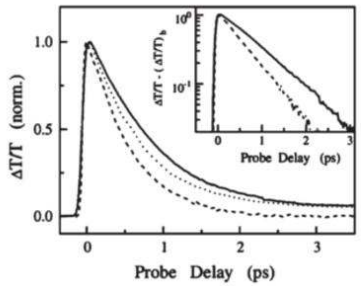
CHEMICAL REVIEWS
REVIEW
pubs.acs.org/CR

Optical Studies of Dynamics in Noble Metal Nanostructures

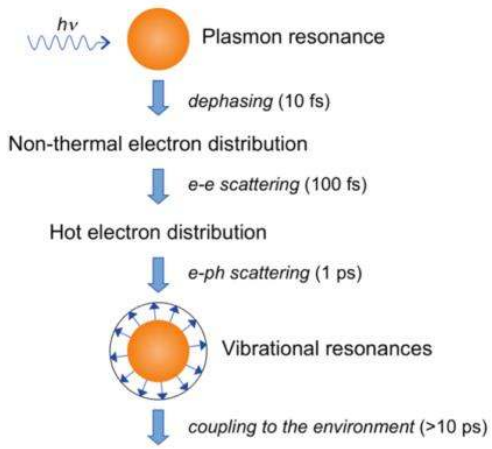
Gregory V. Hartland*

Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, Indiana 46556-5670, United States





Scheme 1. Sequence of Events and Approximate Time Scales Following Absorption of Photons by a Metal Nanoparticle



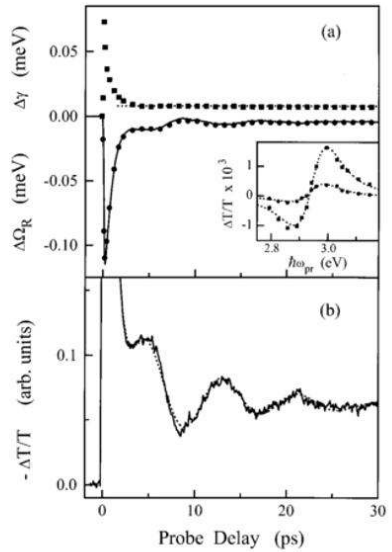
J. Phys. Chem. A 2000, 104, 4321−4326

Acoustic Vibration of Metal Films and Nanoparticles

N. Del Fatti, C. Voisin, D. Christofilos, F. Vallée,* and C. Flytzanis

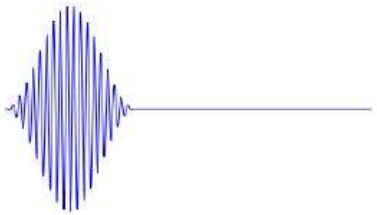
Laboratoire d'Optique Quantique du CNRS, Ecole Polytechnique, 91128 Palaiseau Cedex, France

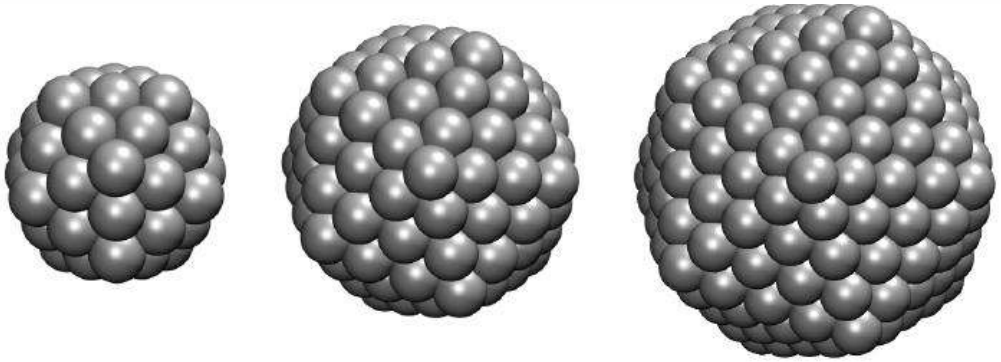
Received: November 16, 1999; In Final Form: January 27, 2000



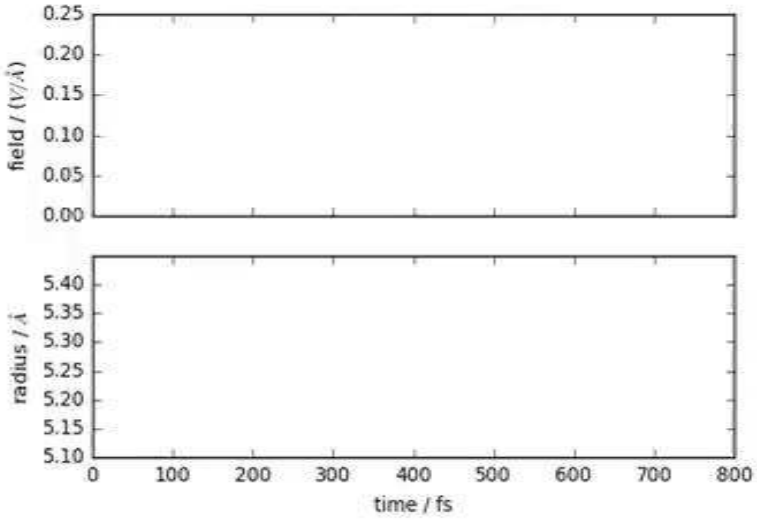
BCCMS

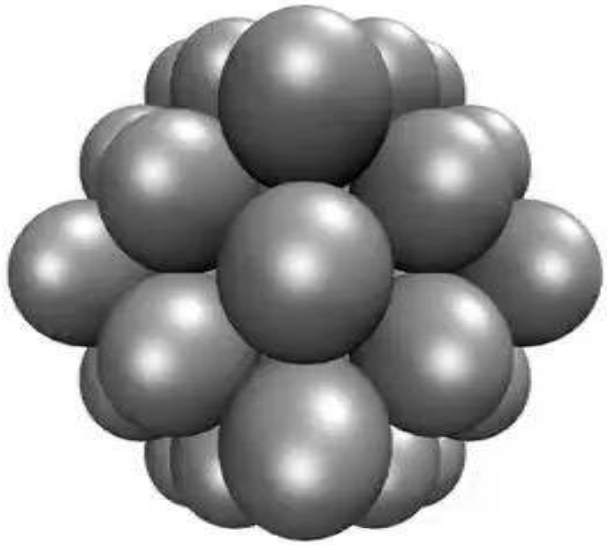
Impulsive breathing mode excitation in Ag and Au NPs





25 fs pulse
frequency tuned to plasmon excitation





Ag: Change in radius versus field strength

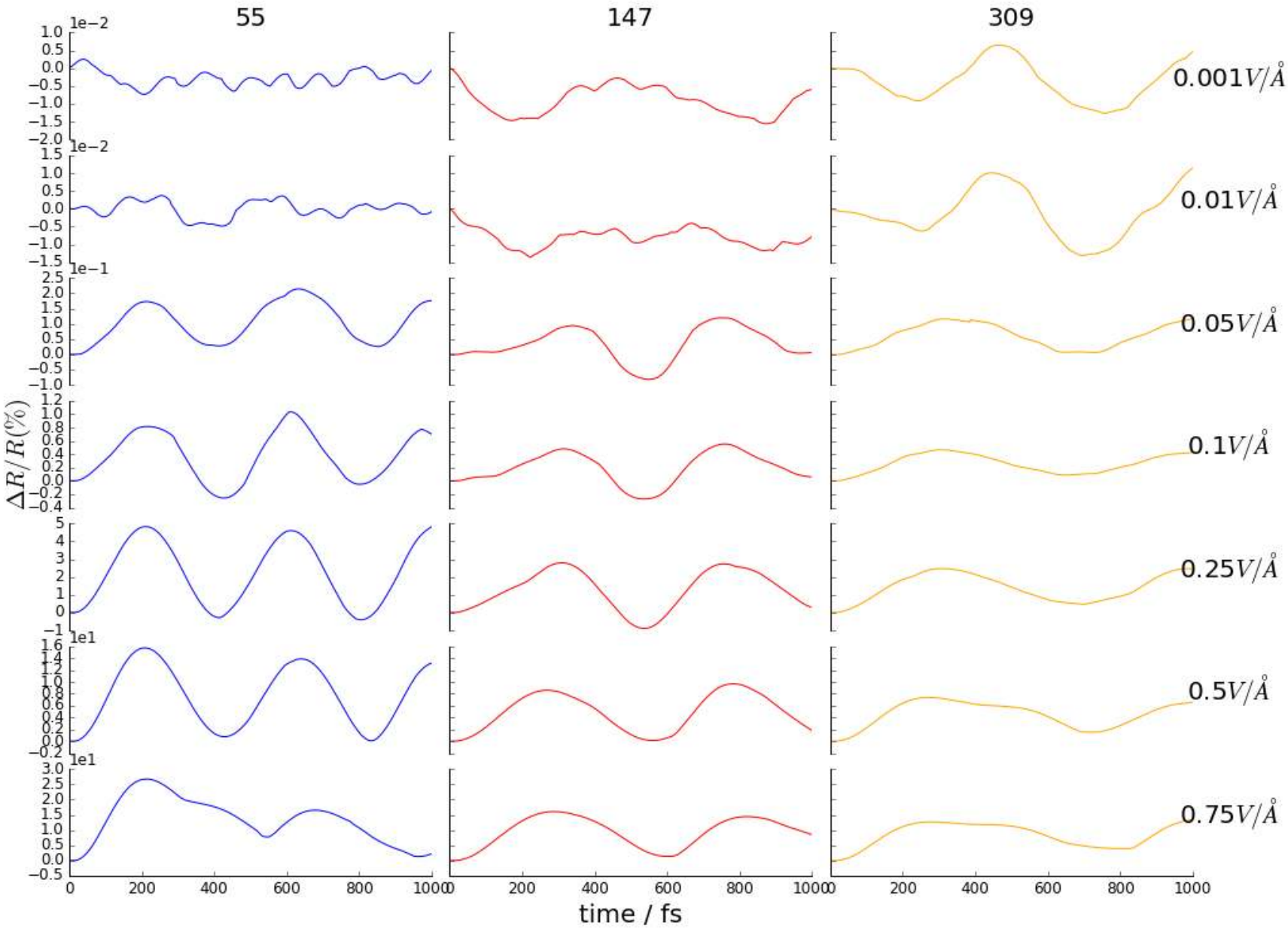
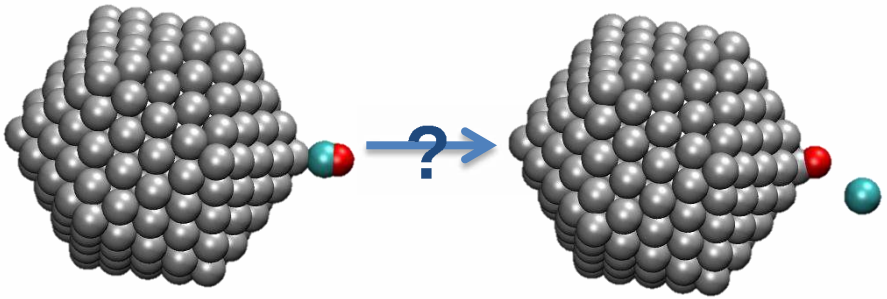
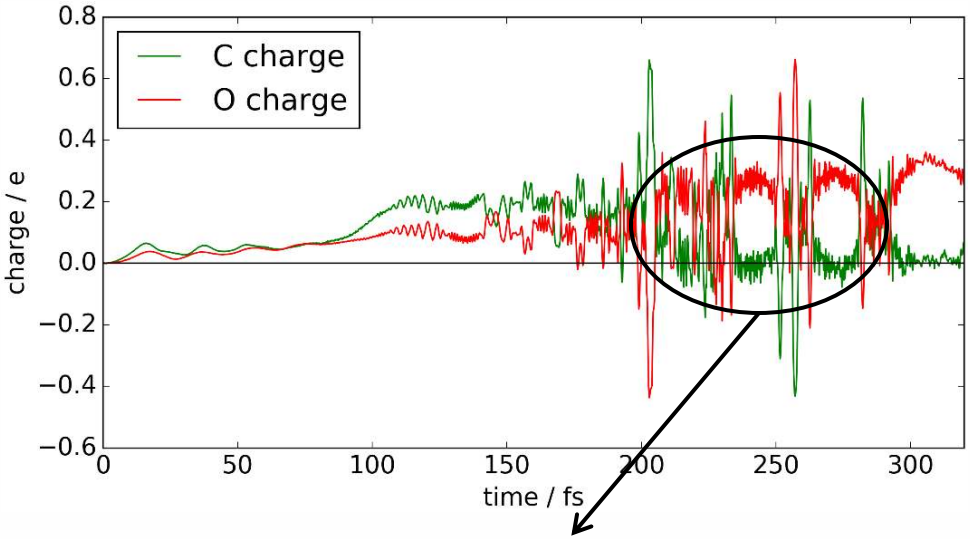


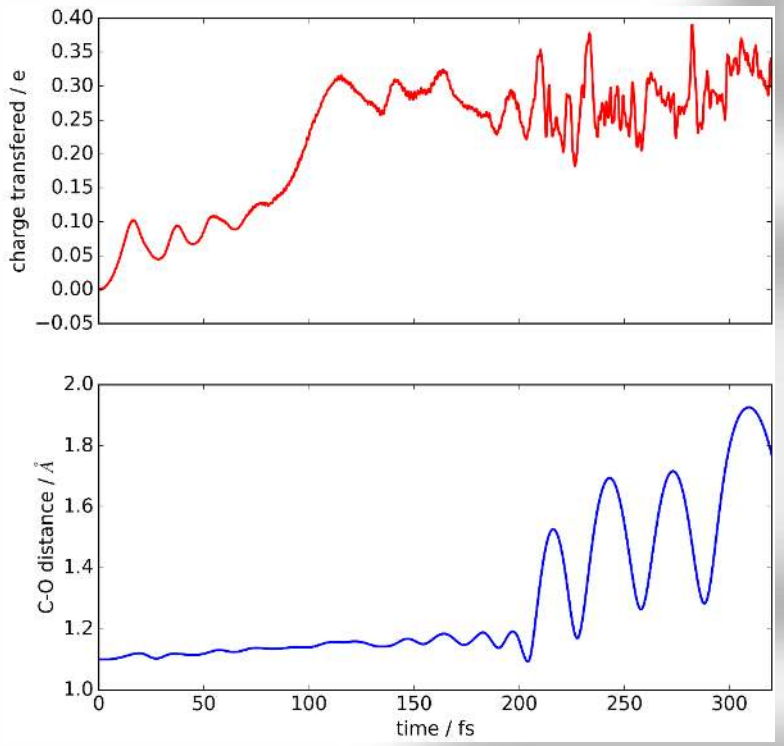
Photo-splitting of CO adsorbed on metal nanoparticles





O holds the negative charge in the antibonding state of CO

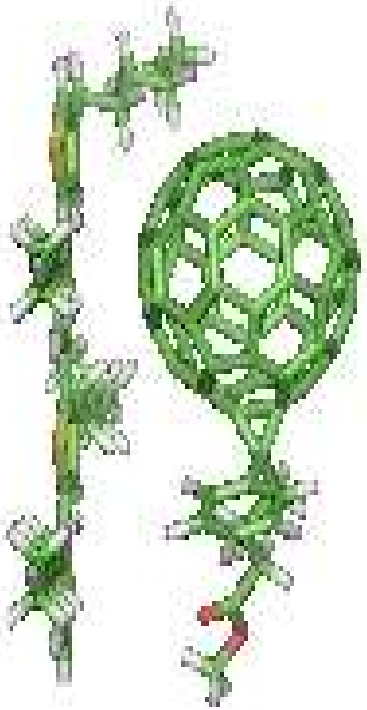
NEW application



Work in progress !

Dynamics of charge separation in organic blends

P3HT - PCBM



Chi Yung Yam

Guanhua Chen

BCCMS

CSRC

Absorption spectra of PCBM and P3HT

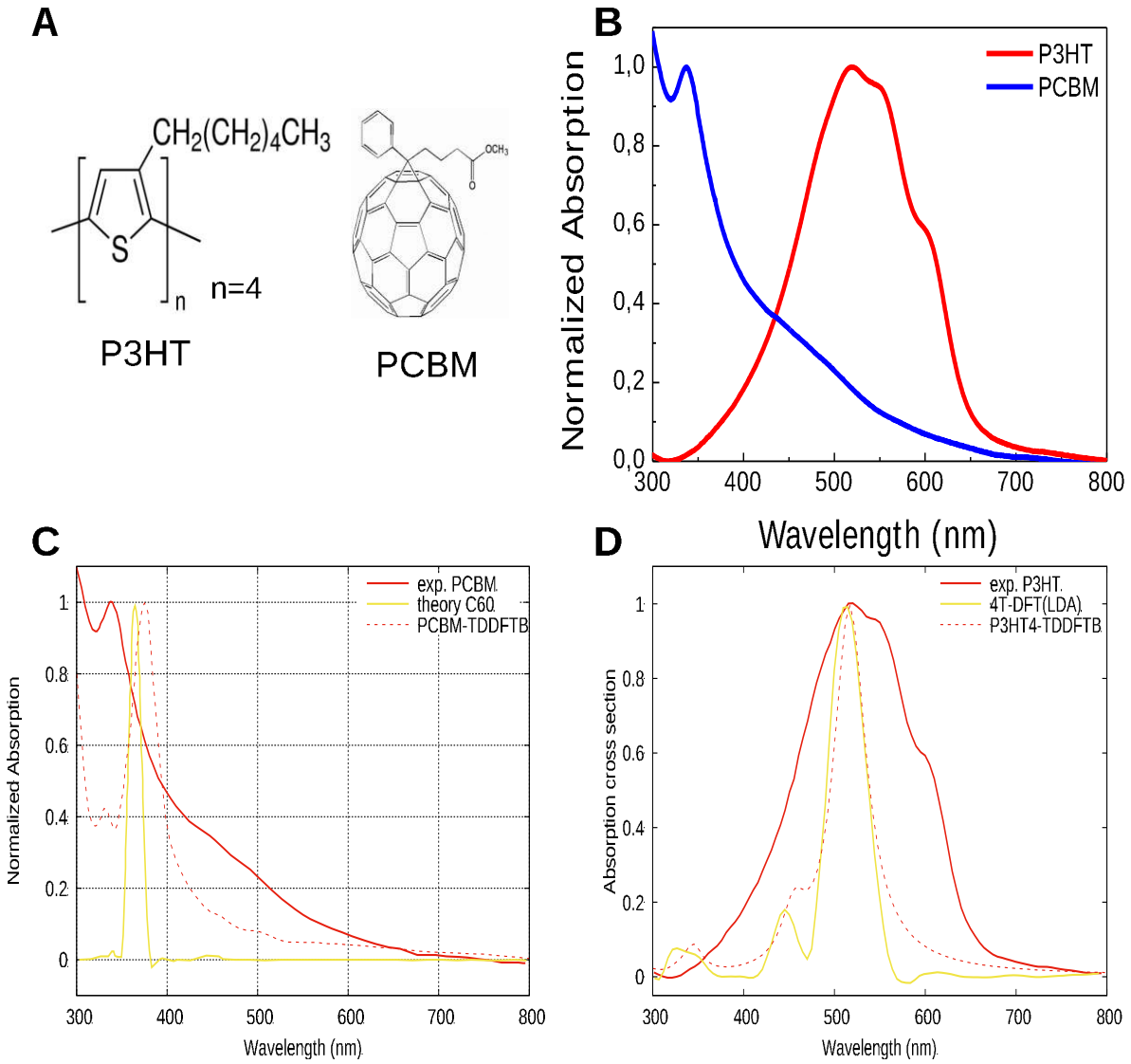
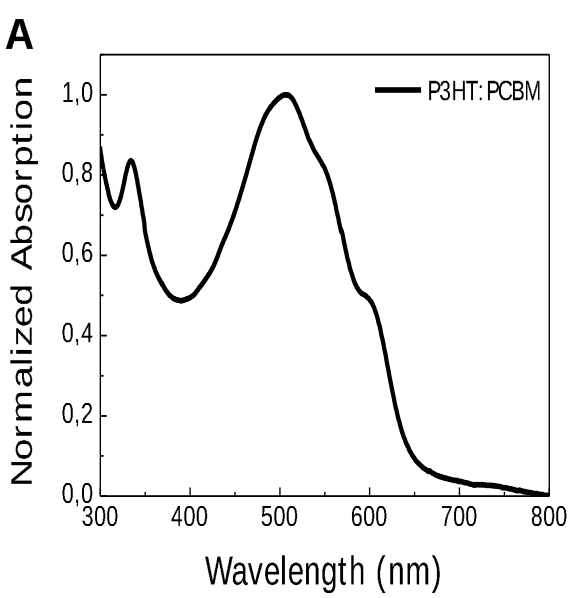
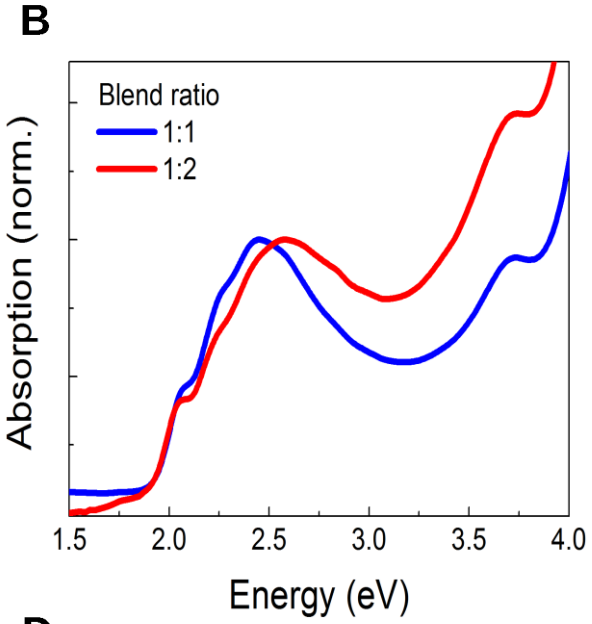
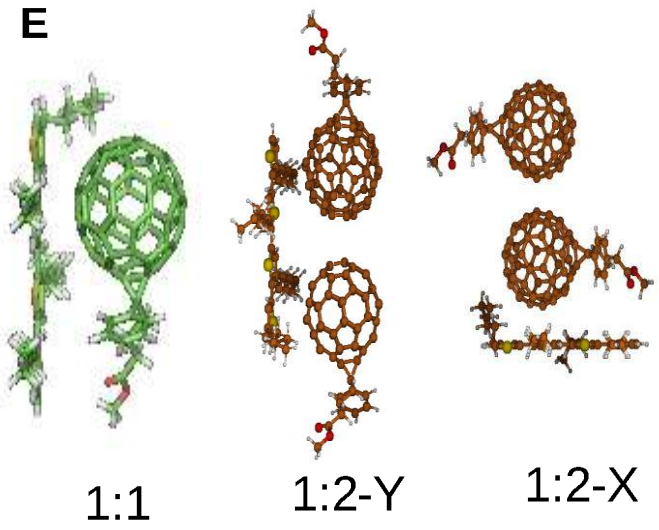


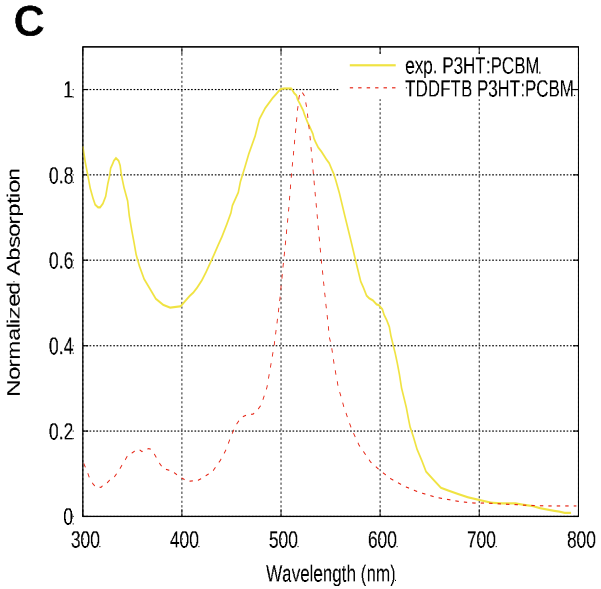
Figure 1 (A) atomic structures of P3HT:PCBM; (B) experiment absorption spectra[1]; (C) absorption spectra of PCBM and (D) absorption spectra of P3HT using TD-DFTB

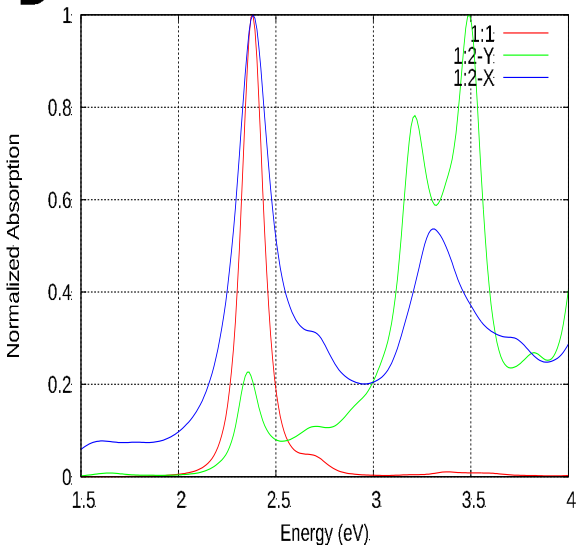
Structures and Absorption Spectra for different aggragation











- 3eV-4eV peak enhancement generated by aggregation of PCBM.

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University
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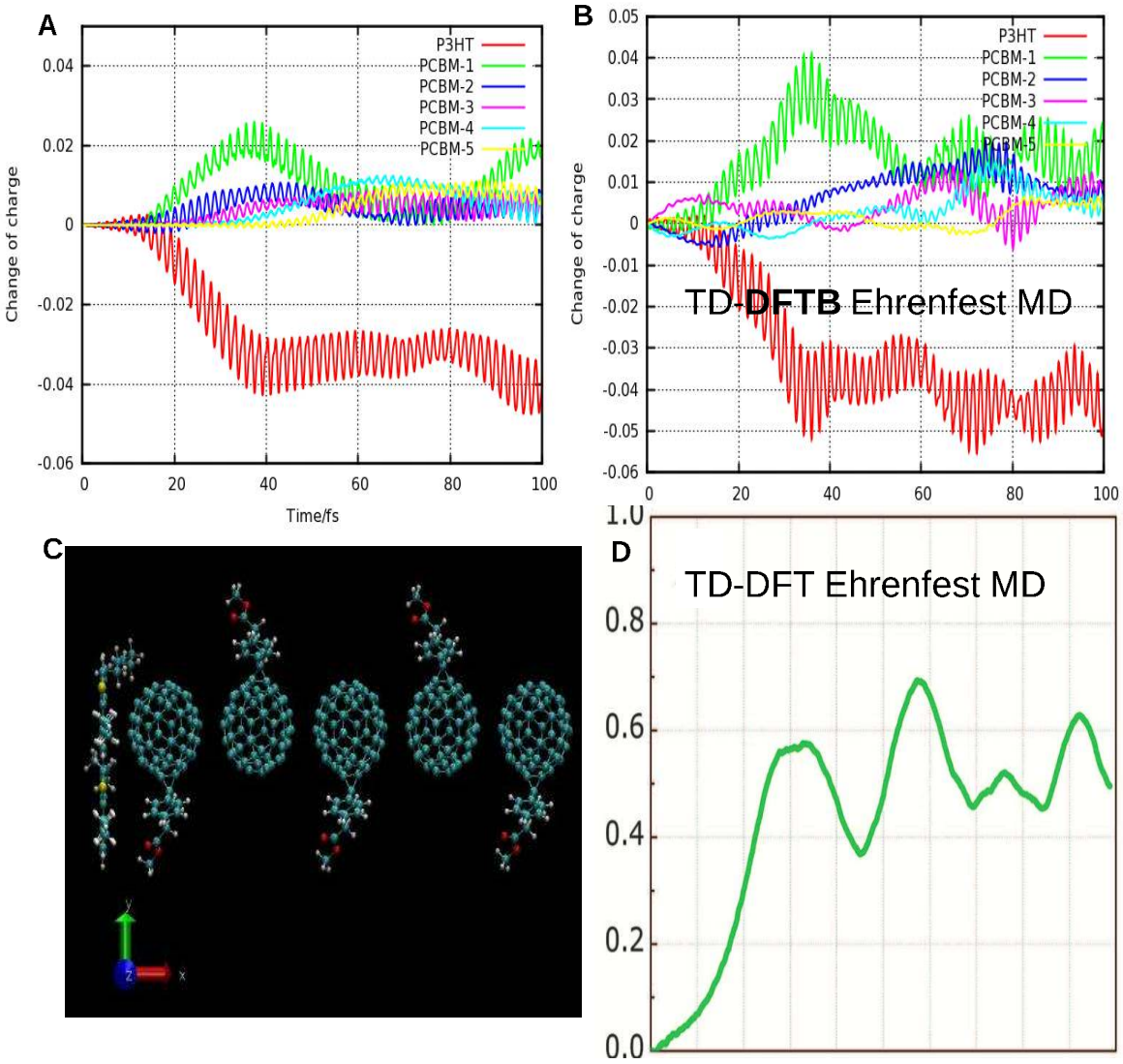
Figure 2 (A) and (B): experiment absorption spectra; (C) and (D): corresponding absorption spectra obtained using TD-DFTB, the atomic structure is shown in (E);

Electron Dynamics with and without Ehrenfest MD



- External field is continuous sine function with frequency corresponding to P3HT absorbance peak;
- External field is applied on P3HT;
- With Ehrenfest, charge transfer process is faster and more charge transfers from P3HT to PCBM;
- The change of charge on P3HT has 20-30fs oscillation which is consistent with TD-DFT Ehrenfest results

Figure 3. The change of charge on molecular fragments without (A) and with (B) Ehrenfest dynamics. The initial velocity is random assigned. (C) Movie of atomic movement with Ehrenfest dynamics. (D) TD-DFT-Ehrenfest result for system containing one P3HT and one PCBM.[1]

Analysis of charge transfer process in multiple layers of P3HT/PCBM

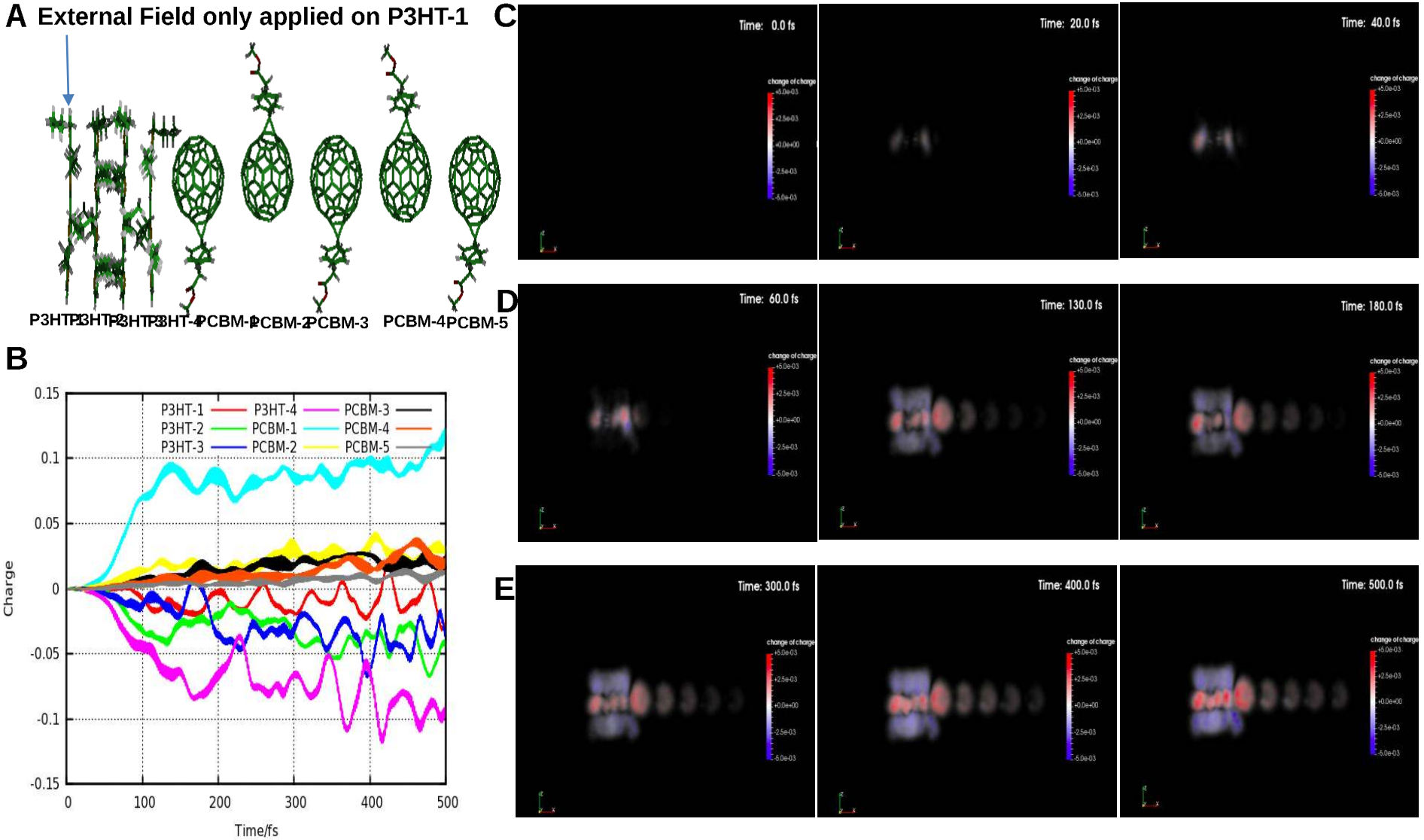
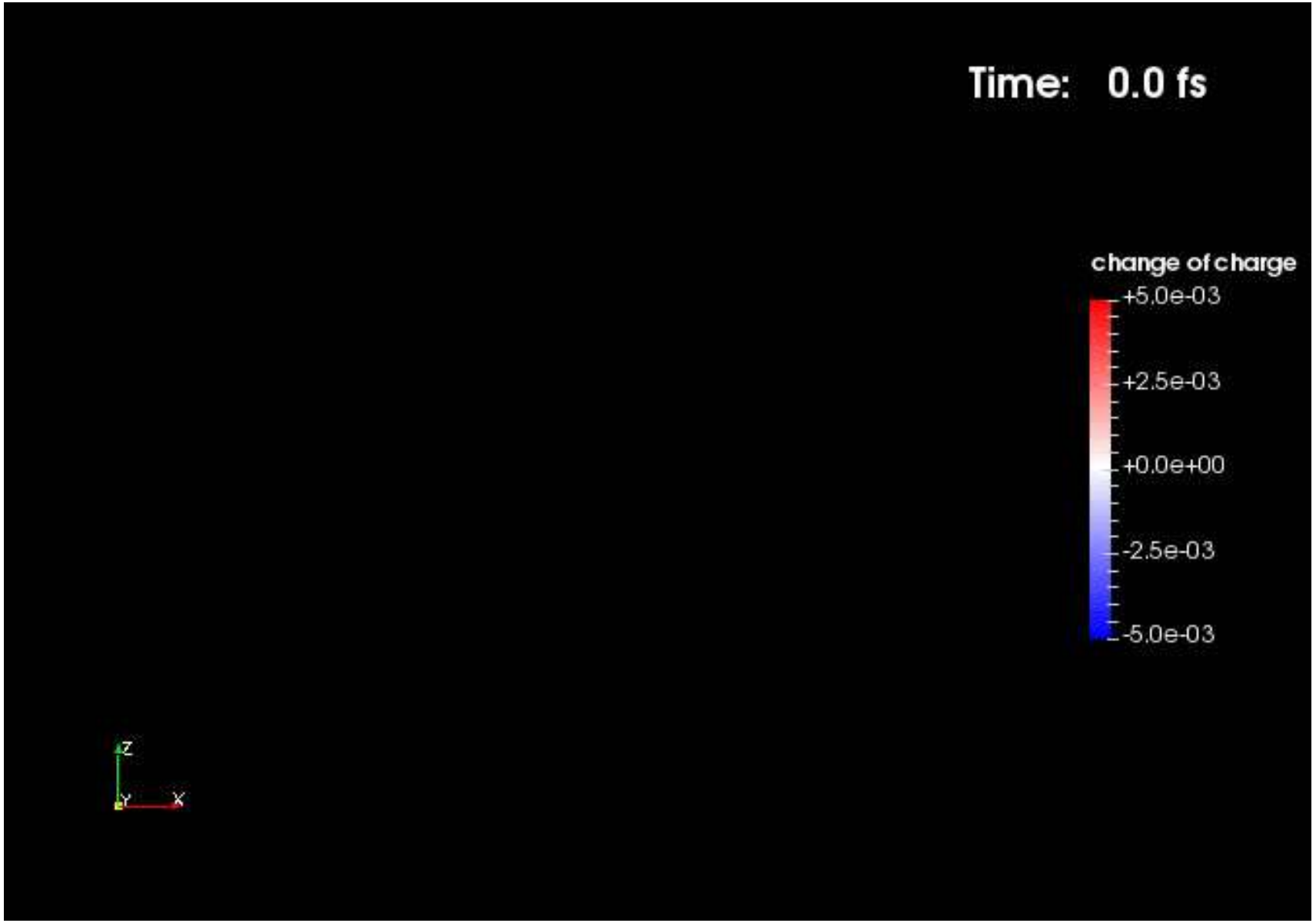


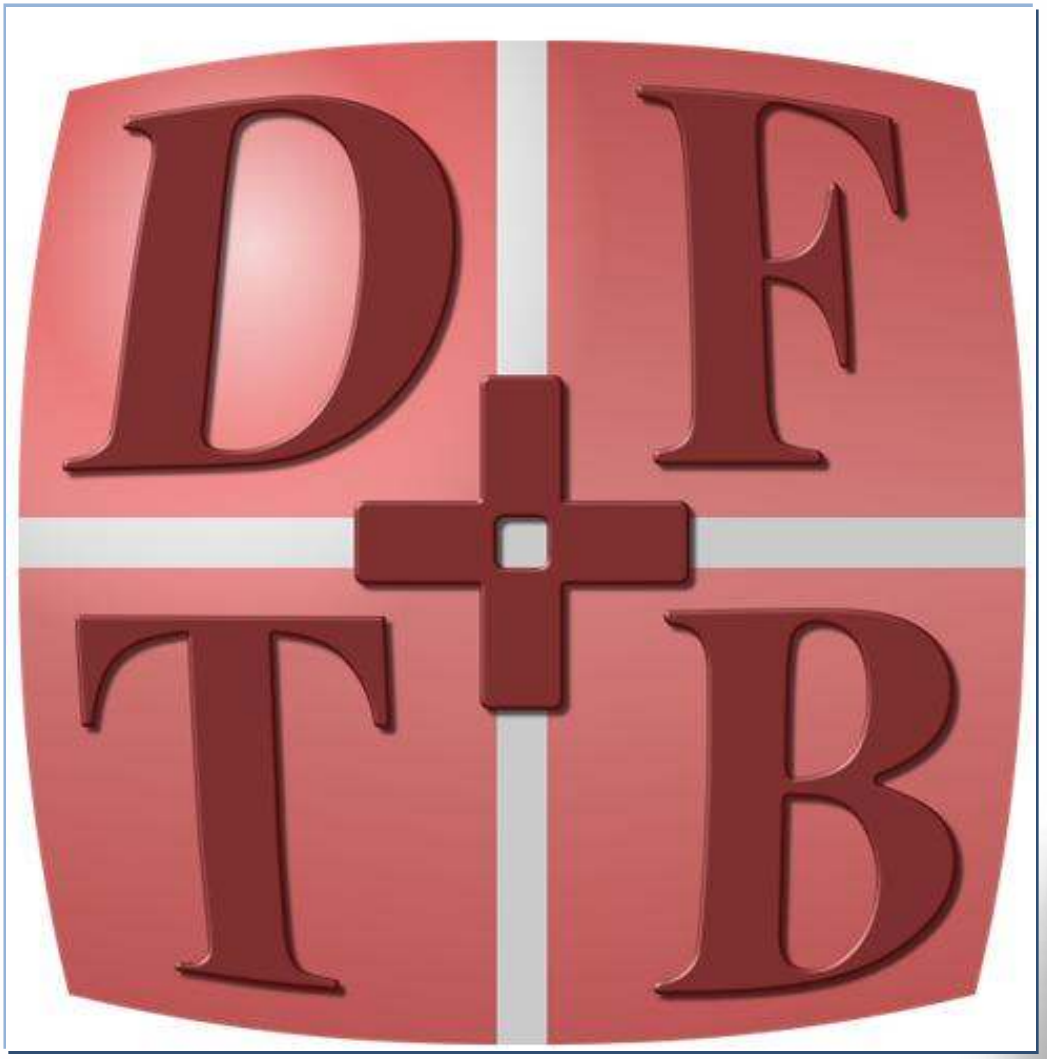
Figure 4 (A) Atomic structure for simulation containing four P3HT and five PCBM aggregates in X direction. (B) The change of charge on each molecular fragments without Ehrenfest; (C,D,E) Snapshots of induced electron density in real space and real time.

Analysis of charge transfer process in multiple layers of P3HT/PCBM

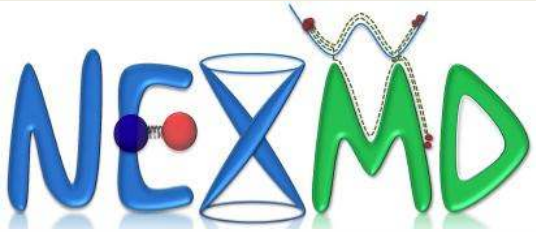


Movie for induced electron density in real space & real time

Summary: DFTB for nanoscale device simulations



DFTB+ connects to world wide software development



Major collaboration partners

Christian Sanchez Cordoba

BCCMS

Bremen Center for Computational Materials Science

http://www.bccms.uni-bremen.de

Acknowledgement – CMS-group

TAB-Building
Technische Akademie Bremen
Am Fallturm 1

Funding agencies: DFG, BMBF, DAAD, AvH, EC,

……

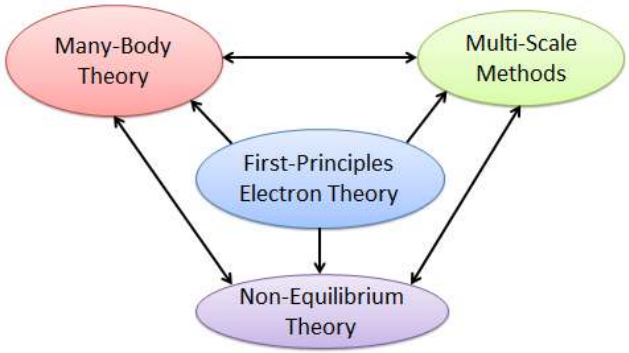
collaborations around the world

Quantum Mechanical Materials Modelling

Research Training Group
DFG - RTG 2247

Speaker/Co-Speaker:
T. Frauenheim; T. Wehling

QM³



Thank You !

Hope to welcome you sometime in Bremen

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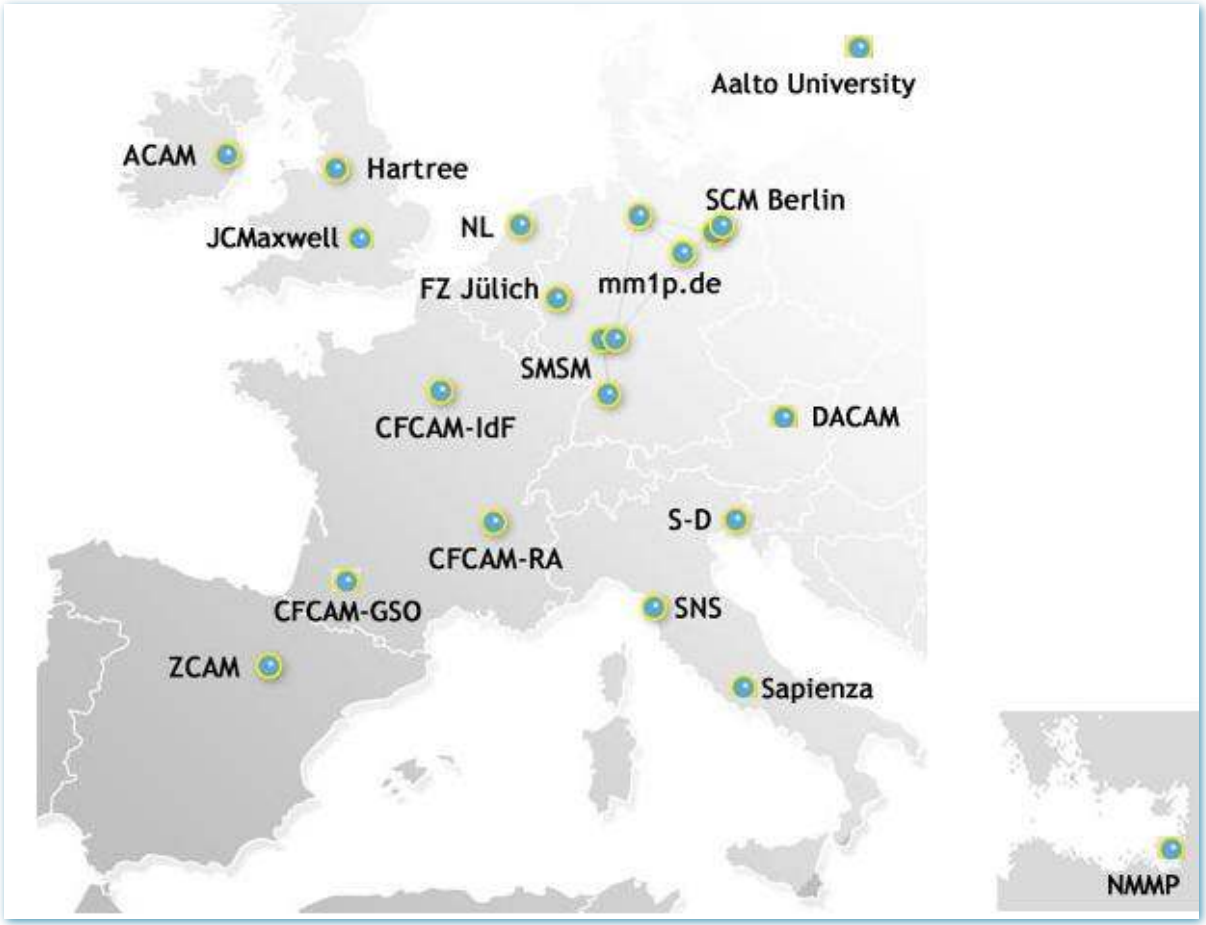
Since 2009 Transformation of CECAM into a multi-nodal structure with CECAM-EPFL as its Headquarter, meanwhile 21 nodes



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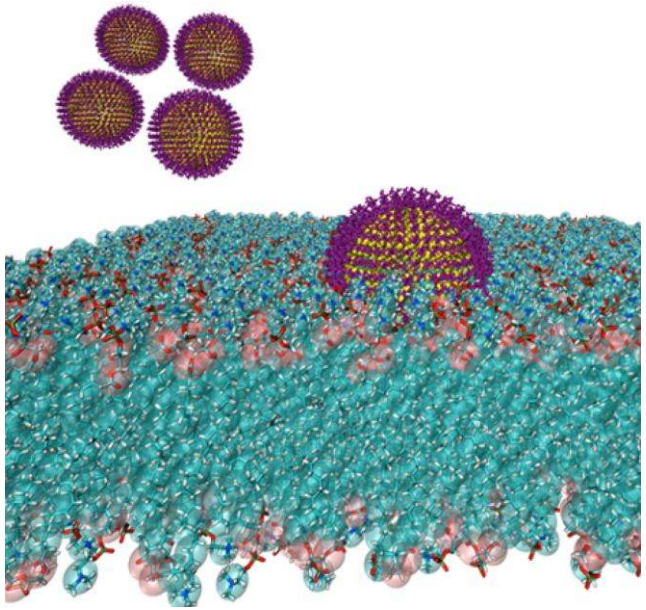

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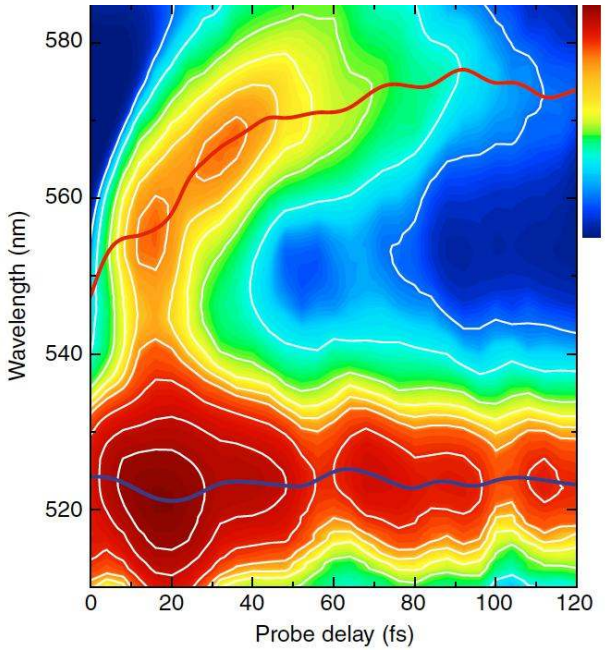

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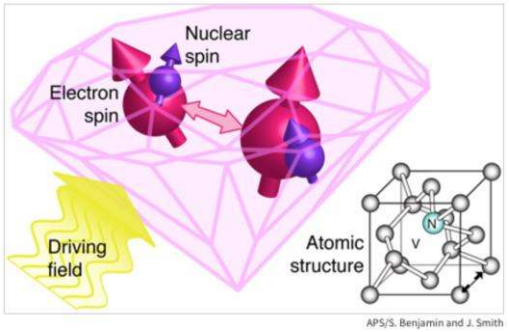
Bremen July 9th to 13th 2018



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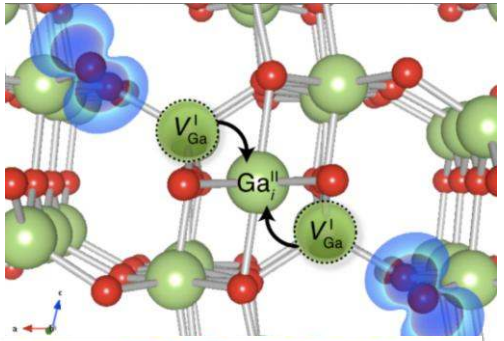

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