



Division Computational & Theoretical Chemistry

**Kick-off meeting:
March 26, 2019
Amsterdam**

The board of the KNCV Division Computational & Theoretical Chemistry (CTC) holds the following people:

Prof. Dr. Matthias (F.M.) Bickelhaupt

VU Amsterdam & Radboud University, Nijmegen (Chair)

Prof. Dr. Célia Fonseca Guerra

Leiden Univ. & VU Amsterdam (Secretary)

Dr. Jörg Meyer

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Amsterdam Center for Multiscale Modeling



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Program

09.00 – 09.10 Opening by Matthias Bickelhaupt (VU)
and Jan-Willem Toering (director KNCV)

chair: Evert Jan Meijer (UvA)

09.10 – 09.55 Paul Geerlings (VUB)

09.55 – 10.25 Bernd Ensing (UvA)

10.25 – 11.05 Coffee and posters

chair: Remco Havenith (RUG)

11.05 – 11.35 Ria Broer (RUG)

11.35 – 12.00 Trevor Hamlin (VU)

12.00 – 12.30 Herma Cuppen (RU)

12.30 – 13.30 lunch and posters

chair: Ad van den Avoird (RU)

13.30 – 14.00 Han Zuilhof (WUR)

14.00 – 14.25 Johannes Klein (RUG)

14.25 – 14.55 Evgeny Pidko (TUD)

14.55 – 15.35 Tea and posters

chair: Peter Bolhuis (UvA)

15.35 – 16.05 Claudia Filipi (UT)

16.05 – 16.30 Ivo Filot (TUE)

16.30 – 16.55 Francesco Buda (LU)

16.55 – 17.00 Awarding of poster prize

17.00 – 17.05 Closure by Célia Fonseca Guerra (VU)
and Jörg Meyer (LU)

17.05 Drinks

ABSTRACTS

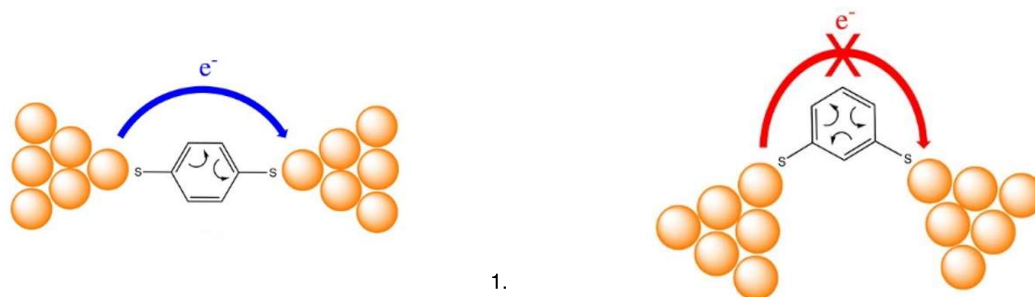
The Linear Response Function in Conceptual DFT: From Mathematical Properties to Applications

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General Chemistry (ALGC), Vrije Universiteit Brussel, Brussels , Belgium

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An overview is given of the work in the ALGC group on the linear response function (LRF), the second functional derivative of the energy with respect to the external potential $v(r)$ at constant number of electrons N , within the context of Conceptual DFT [1-2] Starting from some mathematical properties its physical meaning is highlighted [3-4], and its chemical relevance is shown for interpreting /predicting inductive and mesomeric effects, aromaticity and anti-aromaticity... [5]. Recently addressed topics involving the LRF are discussed [6] such as (1°) the role of the LRF in quantifying Kohn's Nearsightedness of Electronic Matter principle [7,8], (2°) the role of the LRF in the alchemical derivatives approach [9] when exploring Chemical Compound Space [10][11], (3°) the connection between the LRF and single molecule electronics [12][13][14]



1.

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10. R.Balawender, M.Lesiuk, F.De Proft,P.Geerlings,*J.Comp.Chem.Theory* **2018** , 14, 1154

11. R.Balawender, M.Lesiuk,F.De Proft, C.Van Alsenoy, P.Geerlings, to be submitted shortly

12. T.Stuyver,S.Fias,F.De Proft,P.W.Fowler,P.Geerlings,*J.Chem.Phys.* **2015** ,14 , 09410310

13. T.Stuyver, S.Fias, F.De Proft, P.Geerlings, Y.Tsuji, R.Hoffmann, *J.Chem.Phys.* ,**2017**,146 , 092310

14. T.Stuyver,T.Zeng,Y.Tsuji,S.Fias,P.Geerlings,F.De Proft, *J.Phys.Chem.C* , **2018**, 122, 319

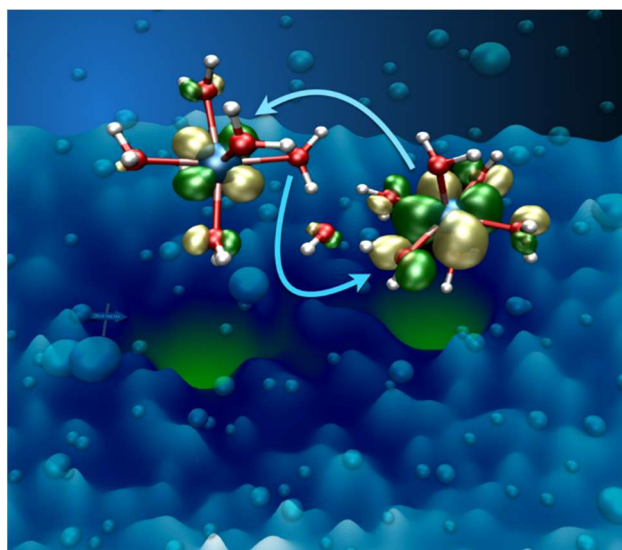
Multiscale simulation of solvent reorganization in charge transport and catalysis

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We combine quantum chemical (DFT) and forcefield molecular dynamics simulations with enhanced sampling techniques to obtain unique insight in the structure and the dynamics of electronic and molecular processes in complex environments [1-4]. We probe for example directly the free energy landscape, from which reaction mechanisms and rates are obtained. In this talk, I will illustrate several recent methodological advancements with examples from catalysis, electrochemistry and enzyme-inspired hydrogen fuel production.



- [1] A. Pérez de Alba Ortíz, A. Tiwari, R. C. Puthenkalathil, and B. Ensing, *J. Chem. Phys.* **2018**, 149, 072320
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- [3] L. Liu, B. Lukose, and B. Ensing *ACS Catalysis* **2018**, 8, 3376
- [4] A Tiwari and B Ensing, *Faraday Discuss.* **2016**, 195, 291

Computation of the dielectric constant and its importance for organic photovoltaics

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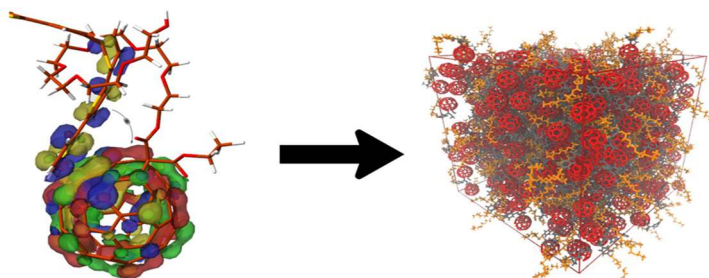
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The current generation of organic photovoltaic (OPV) devices still lacks the required efficiency to be economically competitive. Koster et al. [1] demonstrated that increasing the dielectric constant of organic semiconductors is of key importance for the next-generation of organic photovoltaics.

In this communication, we present a multiscale computational scheme to calculate the different contributions (electronic and nuclear) to the dielectric constant. Our results, for the first time, unravel the timescale of these contributions and shed light on their relevance for high efficiency organic photovoltaics.

The electronic contribution to the dielectric constant can be calculated with high accuracy using the coupled-perturbed Kohn-Sham theory for periodic systems [2]. Nuclear contributions require molecular dynamics simulations, for which a force field specifying all intra- and intermolecular interaction parameters must be defined. Even though there are several readily available standard force fields, it has been shown that these force field parameters fail to reproduce dielectric constants accurately, even for simple organic molecules [3].

An alternative and more powerful approach is to derive these parameters from quantum chemical calculations. However, currently this is also a very time consuming approach: it requires many steps and/or tools to obtain bond, angle, dihedral, charge, polarizability and Lennard-Jones parameters. A single method that can perform all these steps in an automated way, allows for the accurate screening of a large number of molecules using quantum mechanically optimized force fields. With the use of such a method for the generation of polarizable forcefields, we were able to capture both the electronic and nuclear contributions to the dielectric constant and compare the timescale of these contributions to the timescale of recombination mechanisms that occur in OPVs.



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Shasheen, and J.C.

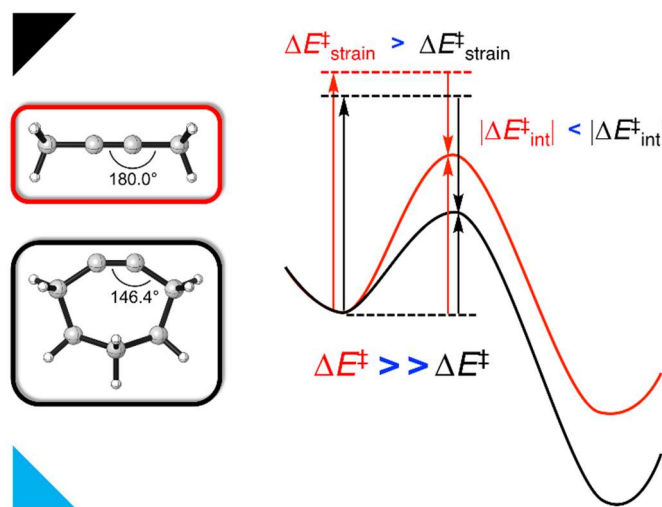
1,3-Dipolar Cycloaddition Reactivity of Alkynes

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The 1,3-dipolar cycloaddition reactivities of acyclic and cycloalkynes were evaluated using density functional theory (DFT) calculations.^[1] Computed activation free energies for the cycloadditions of the acyclic alkyne (2-butyne) are 16-22 kcal mol⁻¹ higher in energy than for the cyclic alkynes. The strained, or pre-distorted nature of cycloalkynes is often solely used to rationalize this significant rate enhancement. Activation strain and bonding analyses have revealed, for the first time, that the degree of the geometrical pre-distortion of the cycloalkyne ground state geometries acts to enhance reactivity compared to acyclic alkynes via three distinct mechanisms: not only due to (i) a reduced strain energy; but also to (ii) a smaller HOMO–LUMO gap; and (iii) an enhanced orbital overlap, which both contribute to a more stabilizing orbital interactions.



[1] T. A. Hamlin, B. J. Levandowski, A. K. Narsaria, K. N. Houk, F. M. Bickelhaupt, *Chem. Eur. J.* **2019**, 25, DOI: 10.1002/chem.201900295.

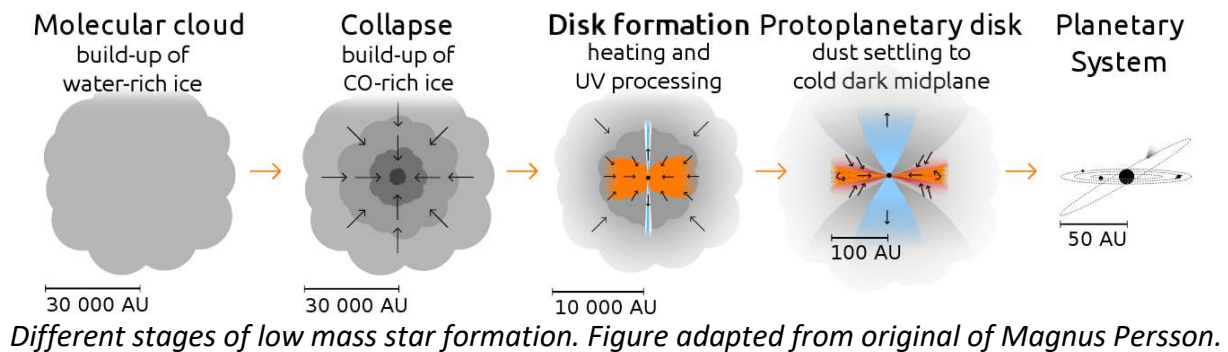
Interactions and dynamics in interstellar ices

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Molecules can form in interstellar clouds despite their low densities and low temperatures. These clouds consist of gas and dust and are the nurseries for stars and planets. Our solar system originated from such a cloud. Molecules play a key role in astrophysical processes, but they also determine the composition of planets, their potential atmosphere and oceans. Of special interest in this respect is the composition of ice mantles that form on top of interstellar dust particles. These ice mantles build up in a time frame of nearly a million years, but are determined by processes on much short time scales. I will show how computational techniques give insight in these different processes and how they can help translate laboratory results to interstellar timescales.



Novel click reactions:

Challenges for both experiment & theory

Jorge Escorihuela,^[a] Jens Looijen,^[a] Adelia Aquino,^[b] Hans Lischka,^[b] Han Zuilhof^[a,b,c]

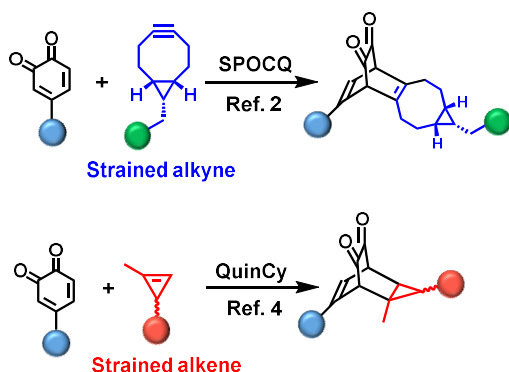
[a] Lab of Organic Chemistry, Wageningen University, Wageningen, The Netherlands. [b] School of Pharmaceutical Science and Technology, Tianjin University, Tianjin, China. [c] Department of Chemical and Materials Engineering, King Abdulaziz University, Jeddah, Saudi Arabia

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Modern synthetic chemistry of both small molecules and complex polymeric materials is increasingly relying on click chemistries: reactions that combine a high yield with smooth, easy-to-apply and environmentally friendly reaction conditions and easy purification and/or high atom efficiency. This combination is quite challenging, but over the last decade more and more candidates have been identified, that function over a wide range of circumstances.^[1,2]

In this search for better reactions, quantum chemical data are often badly needed to make sense of and steer experiments, e.g. in terms of indications of driving force and kinetic bottlenecks. While displaying evident success in some aspects (e.g. the Bickelhaupt-Houk model to obtain the roles of geometrical distortion and reactant interactions on the TS shape and energy),^[3] theory is in others lagging behind. For example, the predictive power of quantum chemistry on multi-phase click reactions, such as those that are surface-bound, is really falling short.^[4]

The goal of this presentation is a) to outline a few of these successful cases of theory-experiment interactions, and b) to indicate a few of the limitations of currently used quantum chemistry, with the aim to further stimulate the interplay of experiment and theory.



The SPOCQ click reaction is ~150x slower when performed at a surface than in dilute solution.

The Quinone-Cyclopropene click reaction only slows down ~4x when surface-bound.

[1] H.C. Kolb, M.G. Finn, K. B. Sharpless, *Angew Chem Int Ed.* **2001**, 40, 2004

[2] D. Gahtory, R. Sen, S. Pujari, S. Li, Q. Zheng, J. E. Moses, K. B. Sharpless, H. Zuilhof, *Chem. Eur. J.* **2018**, 24, 10550

[3] F. M. Bickelhaupt, K. N. Houk, *Angew. Chem. Int. Ed.* **2017**, 56, 10070

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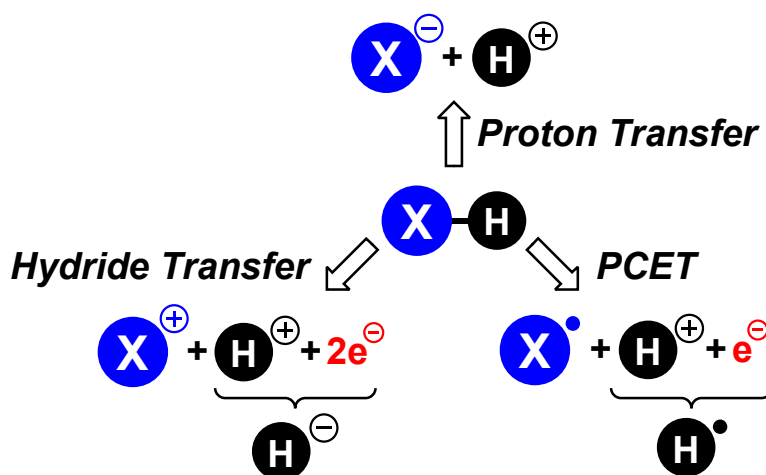
Watching X-H Bonds Break

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The activation of X-H bonds can occur in three distinct ways: (i) proton (H^+) transfer, (ii) proton coupled electron transfer (PCET) (H^+ and e^-) and (iii) hydride transfer (H^+ and $2e^-$). Of these three general pathways, PCET takes a special role as it can follow different scenarios ranging from stepwise to concerted processes.^[1] For the concerted variants either joint transfer of the proton and electron as a true hydrogen atom, often referred to as hydrogen atom transfer (HAT), or separate, yet concerted, transfer of the proton and electron are possible. A fundamental understanding of these events is paramount to developing strategies that control these events in chemical reactions. Such insight can be gained through the use of intrinsic bond orbitals (IBOs),^[2] a type of localized orbitals. Monitoring the changes of IBOs along reaction paths readily identifies the electron flow in chemical transformations.^[3] Applications of this approach to X-H bond activation reactions will be presented demonstrating that this computational tool is clearly capable of differentiating the various scenarios in an intuitive way.^[4]



[1] For reviews see: (a) S. Hammes-Schiffer, *J. Am. Chem. Soc.* **2015**, *137*, 8860; (b) D. R. Weinberg, C. J. Gagliardi, J. F. Hull, C. F. Murphy, C. A. Kent, B. C. Westlake, A. Paul, D. H. Ess, D. G. McCafferty, T. J. Meyer, *Chem. Rev.* **2012**, *112*, 4016; (c) J. J. Warren, T. A. Tronic, J. M. Mayer, *Chem. Rev.* **2010**, *110*, 6961.

[2] G. Knizia, *J. Chem. Theory Comput.* **2013**, *9*, 4834.

[3] G. Knizia, J. E. M. N. Klein, *Angew. Chem. Int. Ed.* **2015**, *54*, 5518.

[4] For examples see: (a) J. E. M. N. Klein, G. Knizia, *Angew. Chem. Int. Ed.* **2018**, *57*, 11913; (b) J. E. M. N. Klein, G. Knizia, L. Nunes Dos Santos Comprido, J. Kästner, A. S. K. Hashmi, *Chem. Eur. J.* **2017**, *23*, 16097.

Breaking linear scaling relationships with secondary interactions: a case study of methane oxidation by di-Fe sites in zeolite and MOF catalysts

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Linear energy scaling relations connect the enthalpies and barriers of key elementary reactions over defined active sites on catalytic surfaces. These relations substantially facilitate a rapid computational catalyst screening, but they also impose fundamental limits on the theoretically attainable activity. Understanding the limits of applicability of the linear scaling relationships is crucial for the development of predictive models in catalysis and pushing the catalytic reactivity beyond the limits set by the intrinsic chemistry of the active site.^[1] Herein, we report a detailed computational study on the mechanism of methane oxofunctionalization^[2] by well-defined Fe complexes in ZSM-5 zeolite^[3] and MOF-type^[4] microporous catalysts. Although the DFT-computed barriers for C-H bond cleavage by Fe-sites in different micropore environment generally scale linearly with the reaction enthalpies and the hydrogen affinities^[5] of the active site, many data-points show substantial deviations from these linear energy relations. We identify three major mechanisms behind these deviations, namely, (1) confinement, (2) multifunctionality and (3) coordinative flexibility. Our computational findings point to the need for the formulation of multidimensional property-activity relationships accounting for both the intrinsic chemistry of the reactive ensembles and secondary effects due to their environmental and dynamic characteristics.

[1] J. Greeley, *Ann. Rev. Chem. Biomol. Eng.* **2016**, 7, 605; L. Grajciar, C.J. Heard, A.A. Bondarenko, M.V. Polynski, J. Meeprasert, E.A. Pidko, P. Nachtigall, *Chem. Soc. Rev.* **2018**, 47, 8307

[2] A.I. Olivos-Suarez, A. Szecsenyi, E.J.M. Hensen, J. Ruiz-Martínez, E.A. Pidko, J. Gascon, *ACS Catal.* **2016**, 6, 2965

[3] A. Szecsenyi, G. Li, J. Gascon, E.A. Pidko, *ACS Catal.* **2018**, 8, 7961

[4] A. Szecsenyi, G. Li, J. Gascon, E.A. Pidko, *Chem. Sci.* **2018**, 9, 6765

[5] A.A. Latimer, A.R. Kulkarni, H. Aljama, J.H. Montoya, J. Suk Yoo, C. Tsai, F. Abild-Pedersen, F. Studt, J. K. Nørskov, *Nat. Mater.* **2017**, 16, 225

“Exciting” news in quantum Monte Carlo

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Quantum Monte Carlo methods are first-principle approaches that provide a stochastic solution to the Schrödinger equation and represent a powerful tool when conventional methods are not reliable. While the methods are routinely employed to predict accurate total energies of relatively large systems, their use is relatively uncommon when coming to excited states and further hampered by the lack of efficient and reliable schemes to obtain energy derivatives. Here, we will illustrate their performance as excited-state methods for prototypical photo-sensitive systems and discuss recent developments which allow the fast and accurate computation of structural properties in quantum Monte Carlo for ground and excited states.

Hierarchical Multiscale Catalytic Modelling: From the active site to the reactor

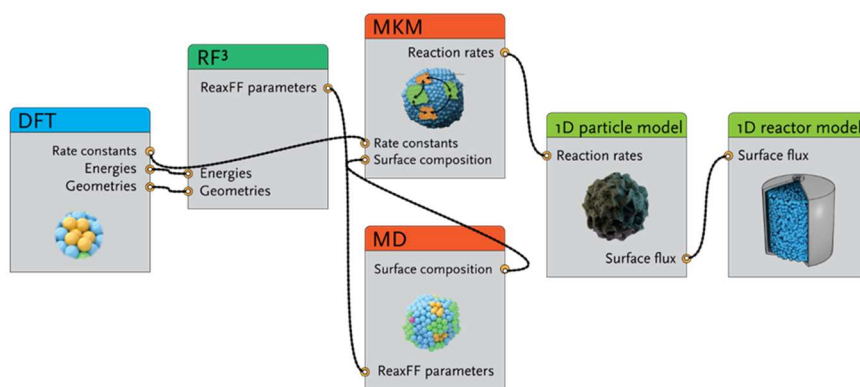
Ivo Filot^[a]

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Rational design of catalytic materials can be achieved using advanced methods that model the multiscale catalyst behaviour from the active site at the nanoscale to the reactor at the macroscale. Such methods are currently rather limited as they lack a proper description of the mesoscale. This leads to oversimplified models, wherein it is typically assumed that the catalytic activity is fully described by a single active site on a single surface facet. Catalytic nanoparticles are composed of many facets, each harbouring one or more active sites that have characteristic activity and selectivity patterns. These active sites are furthermore kinetically linked via diffusion processes over the catalyst nanoparticle and via adsorption/desorption processes with the surrounding gas phase. A proper description of catalytic nanoparticles thus encompasses all these phenomena, which occur on the mesoscale. As this scale is computationally inaccessible at the density functional theory level of theory, models are required that operate at the interplay of sufficient chemical accuracy and feasible computational costs.

In this talk, I will provide a step-by-step introduction how multiscale modelling in heterogeneous catalysis is achieved by using a combination of density functional theory, molecular dynamics, microkinetics modelling and reactor modelling.



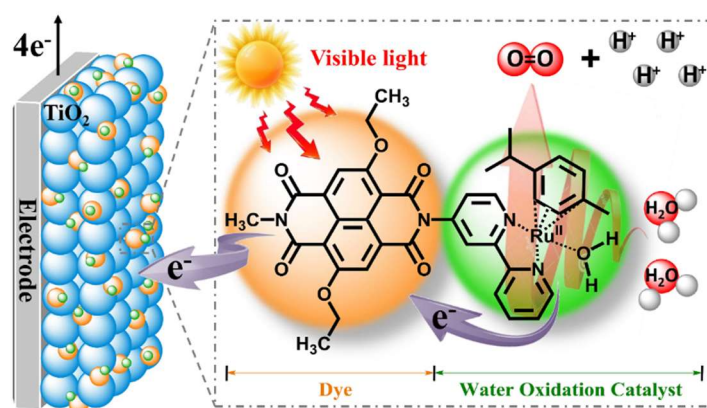
Photocatalytic water splitting for artificial photosynthesis devices

Francesco Buda

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A dye-sensitized photoelectrochemical cell (DS-PEC) is a promising device for direct conversion of solar energy into fuel. The basic idea, inspired by natural photosynthesis, is to couple the photo-induced charge separation process to the catalytic water splitting. The photo-oxidized dye coupled to a water oxidation catalyst (WOC) should exert a thermodynamic driving force for the catalytic cycle, while water provides the electrons for regenerating the oxidized dye. These conditions impose specific energetic constraints on the molecular components of the photoanode in the DS-PEC. Computer simulations and quantum chemical calculations can assist and provide guidelines for the design and optimization of these devices. Here we consider a supramolecular complex integrating a mononuclear Ru-based WOC with a naphthalene-diimide (NDI) dye. It is shown that this dye is able to perform fast photo-induced electron injection into the conduction band of the titanium-dioxide semiconductor anode. Moreover, the oxidized dye is capable of driving the whole photocatalytic water splitting cycle. The results provide strong evidence for the significant role of spin alignment and solvent rearrangement in facilitating the proton-coupled electron transfer processes. The predicted activation energy barriers indicate that the O–O bond formation is the rate-limiting step.^[1-4]



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[2] J.M. de Ruiter, R.L. Purchase, A. Monti, C.J.M. van der Ham, M.P. Gullo, K.S. Joya, M. D'Angelantonio, A. Barbieri, D.G.H. Hetterscheid, H.J.M. de Groot, F. Buda, *ACS Catal.*, **2016**, 6, 7340.

[3] A. Monti, J.M. de Ruiter, H.J.M. de Groot, F. Buda, *J. Phys. Chem. C.*, **2016**, 120, 23074.

[4] Y. Shao, J.M. de Ruiter, H.J.M. de Groot, F. Buda, *to be submitted*.

POSTERS

#	Name	Title
1	Nitish Govindarajan	Modeling Solvent Effects in Catalytic Reactions for Energy Conversion
2	Luis Suarez	Singlet fission materials for enhancing solar cell efficiency: a theoretical study
3	Matthieu	Low-energy scattering resonances as a probe to test the quality of Ab-Initio interaction potentials.
4	Tchakoua Theophile	Towards chemical accurate simulation of dissociation of H ₂ on Ni(111)
5	R.J.P. Broos	Understanding the Fischer-Tropsch reaction on iron carbide surfaces
6	Soroush Rasti	A comparison of empirical force fields and density functional theory for modeling ice
7	Juri Grossi	Functional derivative of the ZPE functional
8	Andrey Konovalov	The Unusual Electrocatalytic Water Oxidation Mechanism by [Cu(Hbbpya)](OTf) ₂
9	Taha Selim	Unraveling Molecular Collisions in Protoplanetary Disks
10	Sivasudhan Rathnachalam	Exploring excited-state dynamics using “on-the-fly” quantum dynamics
11	Bart Klumpers	Machine learning co-adsorbate interactions in catalysis
12	Long Zhang	Activity Trends for CO Oxidation on La Based Perovskite Supported Single Atom Catalysts
13	Sara Giarrusso	Kinetic Energy Density Functional theory for the Continuum
14	R. K. Kathir	Singlet fission studied using non-orthogonal configuration interaction
15	Selim Sami	Computation of the dielectric constant and its importance for organic photovoltaics
16	Stan Papadopoulos	Massively Parallel Implementation of Coupled Cluster Theories in DIRAC using the ExaTensor Library
17	Michel van Etten	The optimal particle size for Co-based Fischer-Tropsch Synthesis
18	Micha Davids	Kinetic Monte Carlo model of methanation on stepped cobalt
19	Tobias Verdonschot	Trends and Analysis of Halide Affinities of the Main Group Elements
20	Kiana Gholamjani Moghaddam	A computational study on the nature of DNA G-quadruplex structure
21	Bart Zijlstra	Microkinetic modeling of the Fischer-Tropsch reaction on metallic cobalt nanoparticles
22	Annika Krieger	Investigating the effect of solvent on transfer hydrogenation mechanisms by homogenous Mn-NN catalyst
23	Pascal Vermeeren	Alkali Cation Catalyzed Diels-Alder Reactions in Space
24	Katharina Doblhoff-Dier	Tackling heterogeneous catalysis with (DFT embedded) diffusion Monte Carlo
25	Chiara Caratelli	Dynamic creation of active sites on UiO-66 by interaction with protic solvents

#	Name	Title
26	Derk Kooi	London dispersion interactions without density distortion
27	Sven Roefs	Dynamic Surface Processes in Cobalt-based Fischer-Tropsch Synthesis
28	Vivek Sinha	The Molecular Basis of Clean Energy
29	Lucas de Azevedo Santos	Benchmark Study of Chalcogen Bonds: An Assessment of DFT functionals
30	Song Yu	Factors Controlling the Diels-Alder Reactivity of Hetero-1,3-Butadienes
31	Tim Jansen	Raising the Temperature on LDFAtom: Electronic Friction at Finite Temperatures
32	Arjun Wadhawan	Understanding Nucleation at Atomistic Scale
33	Alexandre Alves de Castro	Computational and theoretical chemistry in reactivity studies of organophosphorus compounds
34	Hans de Bruijn	Hydroaminomethylation with a Co-based catalytic system: understanding hydrogenation selectivity with DFT calculations
35	Jittima	Theoretical study of CO ₂ hydrogenation on Cd ₄ /TiO ₂ catalyst
36	Daniela Rodrigues Silva	Evaluation of the gauche effect in 2-fluorocyclohexanone analogues: an NMR and DFT study
37	Alice Cuzzocrea	A stochastic route to an efficient and accurate description of photo-excitations
38	Rakesh Chandran	Linear scaling relationship to predict the pK _a of [FeFe] hydrogenase enzyme mimics
39	Bruno Senjean	Gradient calculation for quantum chemistry on near-term quantum computers
40	Chandan Kumar	Implementation of theoretical methods for VCD including low-lying excited states
41	Souloke Sen	Environmental Effects on the UV-Vis Spectra of Chlorophyll in the LHCII complex
42	Jelena Belic	Computational optimization of light absorbing dye for the production of solar fuels
43	Eugene Gvozdetzky	Variational vs. perturbative spin-orbit approaches
44	Johann Pototschnig	Revisiting the Canonical Product Format for Full Configuration Interaction
45	Jonas Feldt	A Perturbative Monte Carlo QM/MM Study of Molecular Systems in Solution
46	Narges Asadi-Aghbolaghi	Plasmon Excitation for Pure and Bimetallic Au-Ag Cluster by TD-DFT based Tight Binding
47	Yang Shao	A Strategy for lowering the O–O Bond Formation Energy Barrier in Photocatalytic Water Splitting: Introducing a Proton Acceptor near the Active Site
48	Jan Paul Menzel	Photoinduced electron injection into a dye-sensitized Titanium Dioxide Electrode
49	Eva J. Meeus	Computationally aided rational design of GQ-ligands
50	Hugo Beks	Proton affinity of water from Density Functional Theory based Molecular Dynamics.



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