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Publication List

1 K.L. Jimenez-Monroy, N. Renaud, J. Drijkoningen, D. Cortens, K. Schouteden, C. v Haesendonck, W. J. Guedens, J. V. Manca, L.D.A Siebbeles, F.C. Grozema, P.H. Wagner *High Electronic Conductance through Double-Helix DNA Molecules with Fullerene Anchoring Groups*,
J. Phys. Chem. A., article ASAP, DOI: 10.1021/acs/jpca.7b00348, **2017**

2 J. Lauth, A. Kulkarni, F. C. M. Spoor, N. Renaud, F. Grozema, A. J. Houtepen, J. M. Schins, S. Kinge, L. D. A. Siebbeles *Photogeneration and Mobility of Charge Carriers in Atomically Thin Colloidal InSe Nanosheets Probed by Ultrafast Terahertz Spectroscopy*,
J. Phys. Chem. Lett., **7**, 4191-4196 **2016**

3 N. Renaud, M. A. Harris, A. P. N. Singh, Y. A. Berlin, M. A. Ratner, M. R. Wasielewski, F. D. Lewis, and F. C. Grozema *Deep-Hole Transfer Leads to Ultrafast Charge Migration in DNA Hairpins*,
Nature Chemistry, **8**, 1015-1021 **2016**
Highlighted in Nature Chem. News and Views **8**, 992 - 993 **2016**

4 R. Frisenda, V.A.E.C Janssen, F. C. Grozema, H. S. J. van der Zant and N. Renaud *Mechanically Controlled Quantum Interference in individual π-Stacked Dimers*,
Nature Chemistry, **8**, 1099-1104, **2016**
Cover Article

5 M.C. Gelvez-Rueda, D. H. Cao, S. Patwardhan, N. Renaud, C. C. Stoumpos, G. C. Schatz, J. T. Hupp, O. K. Fartha, T. J. Savenije, M. G. Kanatzidis,, F. C. Grozema, *Effect of Cation Rotation on Charge Dynamics in Hybrid Lead Halide Perovskites*, J. Phys. Chem. C, *Article ASAP*, J. Phys. Chem. C, **120**, 16577-16585, **2016**, DOI: 10.1021/acs.jpcc.6b06722

6 F. Pietra, L. de Trizio, A. Hoekstra, N. Renaud, M. Prato, F. C. Grozema, P. Baesjou, R. Koole, L. Manna, A. Houtepen *Tuning the Lattice Parameter of InxZnyP for Highly Luminescent Lattice-matched core/shell Quantum Dots*,
ACS Nano, **10**, 4754-4762, **2016**

7 N. Gorczac, N. Renaud, E.Galan, R. Eelkema, L.D.A Siebbeles, F.C. Grozema *Computational design of donor-bridge-acceptor systems exhibiting pronounced quantum interference effects*,
Phys. Chem. Chem. Phys. **18**, 6773-6779, **2016**

8 F. C. M. Spoor, L. T. Kunneman, W. H. Evers, N. Renaud, F. C. Grozema, A. J. Houtepen and L. D. A. Siebbeles*High Energy Optical Transitions in PbSe Quantum Dots: Assignment and Application for Disentangling Electron and Hole Relaxation*,
ACS Nano **10**, 695-703, **2015**

9 Y. Zhang, R. M. Young, A. K. Thazhathveetil, A. P. N. Singh, C. Liu, Y. A. Berlin, F. C. Grozema, F. D. Lewis, M. A. Ratner, N. Renaud, K. Siriwong, A. A. Voityuk, M. R. Wasielewski, and D. N. Beratan, *Conformationally Gated Charge Transfer in DNA Three-Way Junction*,
J. Phys. Chem. Lett., **6** 2434-2438, **2015**

10 N. Gorczak, N. Renaud, S. Tarkuc, A. J. Houtepen, R. Eelkema, L. D. A. Siebbeles, F. C. Grozema
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Chem. Sci., **6** 4196-4206, **2015**
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11 R. M. Young, A. P. N. Singh, A. K. Thazhathveetil, V. Y. Cho, Y. Zhang, N. Renaud, F. C. Grozema, D. N. Beratan, M. A. Ratner, G. C. Schatz, Y. A. Berlin, F. D. Lewis, M. R. Wasielewski,
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Intermolecular Vibration Modes Speed Up Singlet Fission in Perylenediimide Crystals,
J. Phys. Chem. Lett., **6**, 360-365 **2015**

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Phys. Rev. B, **90**, 165307, **2014**

14 M. L. Perrin, R. Frisenda, M. Koole, J. S. Seldenthuis, J. A. Celis Gil, H. Valkenier, J. C. Hummelen, N. Renaud, F. C. Grozema, J. M. Thijssen, D. Dulić and H. S. J. van der Zant,
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Nature Nano., **9**, 830-834, **2014**

15 F. Mirjani, N. Renaud, N. Gorczak, and F. C. Grozema,
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J. Phys. Chem C, **118**, 14192-14199, **2014**

16 N. Gorczak, S. Tarkuç, N. Renaud, A. J. Houtepen, R. Eelkema, L. D. A. Siebbeles F. C. Grozema,
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J. Phys. Chem. A, **118** 3891-3898, **2014**

17 N. Renaud, Y. A. Berlin, M. A. Ratner,
Impact of a single base pair substitution on the charge transfer rate along short DNA hairpins,
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18 N. Renaud, F. D. Lewis, Y. A. Berlin, M. A. Ratner,
Between Superexchange and Hopping: An Intermediate Charge-Transfer Mechanism in Poly(A)-Poly(T) DNA Hairpins,
J. Am. Chem. Soc. **135**, 3953-3963, **2013**

19 J. Iehl, M. Frasconi, H-P Jacquot de Rouville, N. Renaud, S. M. Dyar, N. Strutt, R. Carmieli, M. R. Wasielewski, M. A. Ratner, J-F Nierengarten and J. F. Stoddart,
Dimerization of Viologen Subunits around the C60 Core : From Twelve to Six Directions,
Chem. Sci. **4**, 1462,1469, **2013**

20 M. Zarea, N. Renaud, D. Powell, B. Moghavar, M. R Wasielewski, M. A. Ratner,
Decoherence and Quantum Interference in a Four-Site Model System: Mechanisms and Turnovers,
J. Phys. Chem B, **117**, 101,1020, **2013**

21 N. Renaud, P. Sherrat, M. A. Ratner
Mapping the relation between stacking geometries and singlet fission yield in a class of organic crystals,
J. Phys. Chem. Lett, **4** 1065-1069, **2013**

22 N. Renaud, D. Powell, M. Zarea, B. Moghavar, M. R Wasielewski, M.A. Ratner
Quantum interference and electron transfer in Photosystem I,
J. Phys. Chem. A **117**, 5899-5908, **2013**

23 N. Renaud, C. Joachim,
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24 C. Joachim, N. Renaud, M. Hliwa,
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Adv. Mat. **24** 312-317 **2012**

25 N. Renaud, V. Mujica, M. A. Ratner,
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26 J. Hutcheston, I. Franco, N. Renaud, M. Carignano, M. A. Ratner, G. C. Schatz, *TRANSpull: computes pulling coupled to transport properties of single molecules*, https://nanohub.org/resources/transpull. DOI: 10.4231/D3MP4VN2Z, **2011**

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Phys. Chem. Chem. Phys. **13**, 14404 **2011**

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Phys. Rev. B, **83**, 155443 **2011**

29 N. Renaud, M. Hliwa, Christian Joachim,
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30 N. Renaud, M.A. Ratner, Christian Joachim,
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J. Phys. Chem. B, **115**, 5582 **2011**

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Classical Boolean logic gates with quantum systems,
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ACS Nano, **5**, 1436, **2011**

33 N. Renaud
Calculateur Quantique Hamiltonien, vers une analyse symbolique des circuits quantiques, Editions Universitaires Europeennes, ISBN : 978-613-1-52927-6, **2011**

34 N. Renaud, M. Ito, W. Yang, M. Saeys, M. Hliwa, C. Joachim,
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Chem. Phys. Lett. **472**, 74-79, **2010**

35 I. Duchemin, N. Renaud, C. Joachim,
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Chem. Phys. Lett, **452**, 269-274, **2008**

36 N. Renaud, C. Joachim,
Design and Stability of NOR and NAND logic gates constructed with three quantum states,
Phys. Rev. A, **78** 062316, **2008**

37 N. Renaud, P. Solinas, R. Mosseri, C. Joachim,
Geometrical Approach of Quantum Hamiltonian Computer,
E-Nano newsletter, **8**, 5-10, **2007**

Selected Oral Communications

Faculty Colloquium, Laval University
15th March **2016**, Quebec City, Canada *Invited Presentation*
Controlling Charge Transfer at the Single Molecule Level

International Conference on Perovskite Thin Film Photovoltaics,
2-4 march **2016**, Barcelona, *Contributed Presentation*
Interplay between dipole organization and electronic properties in halide perovskites

FOM Workshop on Quantum Interference,
28 January **2015**, Delft, *Invited Presentation*
Electronic Quantum Interference in Donor-Bridge-Acceptor Molecules

Physics at FOM, The Dutch Physics Conference,
20-21 January **2015**, Veldhoven, *Contributed Presentation*
Intermolecular Vibration Modes Speed-up Singlet Fission in PDI crystals

Faculty Colloquium, McGill University
8th December **2014**, Montreal Canada *Invited Presentation*
Controlling Charge Transfer at the Single Molecule Level

CHAIN, The Dutch Chemistry Conference,
17-18 November **2014**, Veldhoven, *Contributed Presentation*
Mechanical Control of Quantum Interference in π-stacked Molecular Dimer

Gordon Conference on Charge Transfer in Donor-bridge-acceptor Systems
3-8 August **2014**, Newport, *Poster Presentation*
Multiscale Molecular Simulations of Hole Transfer in DNA Hairpins

Faculty Colloquium, Delft University of Technology,
16th August **2014**, Delft, *Invited Presentation*
Multiscale Molecular Simulation for Chemical Engineering

Faculty Colloquium, Leiden University,
15th April **2014**, Leiden, *Invited Presentation*
Controlling Charge Transfer at the Single Molecule Level

12th European Conference on Molecular Electronic
3 – 7 September **2013**, Imperial College London, *Poster Presentation*
Quantum Interference and Spin Properties of Organic Radical in Break Junctions

Modeling Single-Molecule Junctions: Novel Spectroscopies and Control
14 - 16 Oct. **2013**, Fritz Haber Institute, Berlin, *Poster Presentation*
Quantum Interference and Spintronic in mechanically break junctions

Amsterdam Density Functional Developers Workshop,
18-20 February **2013**, Amsterdam, *Invited Presentation*
Singlet Fission and Charge Transfer, Density Matrix Propagation

Les Houches Physics Winter School, Quantum resources and molecule-machines
27 Jan - 01 Feb **2013**, Les Houches, France, *Invited Lecturer*
6 hours of lectures on theoretical methods for molecular studies

AtMol International Workshop on Molecular Machine
23-27 January **2012**, Barcelona, Spain, *Invited Presentation*
Quantum Hamiltonian Computer a symbolic analysis of quantum circuits

QuEBS: Workshop on Quantum Effects in Biological Systems
June 4-6 **2012** , Berkeley, CA, USA, *Invited Presentation*
Quantum Interference in Photosystem I

CIFAR meeting, Nanoelectronic Devices,
April **2010**, Nappa Valley CA, USA *Invited Presentation*
Single Molecular devices, from classical to quantum design