# Nicolas Renaud

Section Head Natural Science & Engineering · Netherlands eScience Center

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## Work Experience

**Netherlands eScience Center** Amsterdam, The Netherlands

Section Head - Natural Science & Engineering *June 2021 - Present*

- Line manager of 15 research software engineers
- Scientific advisor on 20 projects
- Project lead on 7 projects
- Research topics : Material Science, Quantum Chemistry, Quantum Computing

Research Manager - Computational Science for Energy Research *Feb 2018 - May 2021*

- Line manager of 6 - 10 research software engineers
- Project coordinator of 8 projects
- Lead engineer on 4 projects
- Research topics : Material Science, Energy research, Quantum Chemistry

Senior Research Software Engineer *Aug 2017 - Jan 2018*

Research topic: Machine learning methods for protein-protein interface ranking

**Delft University of Technology - Chemical Engineering Department** Delft, The Netherlands

Post Doctoral Researcher *Feb 2013 - Jun 2017*

- Research topics: Quantum chemistry for energy and charge transfer in molecular systems
- Teaching: Main Lecturer for MSc course Numerical techniques for chemical engineering (Best teacher of the year nomination)
- Supervisor: Prof. Ferdinand Grozema

**Northwestern University - Theoretical Chemistry Department** Evanston, Illinois, USA

Post Doctoral Researcher *Jan 2010 - Dec 2012*

- Research topics: Quantum transport in single molecules
- Supervisor: Prof. Mark Ratner

## Education

**PhD in Nanoscience** Université Paul Sabatier & CEMES - CNRS *Sept. 2006 - Nov. 2009*

- Thesis: Quantum Hamiltonian Computing : From theory to experiments.
- Research topics: quantum transport, quantum logic gates, quantum chemistry.
- Supervisor: Dr. Christian Joachim

**MSc in Nanoscience** Université Paul Sabatier *Sept. 2005 - Aug. 2006*

- Master Thesis: Quantum Hamiltonian Computing
- Supervisor: Dr. Christian Joachim

## Open Source Packages

**QMCTorch** Quantum Monte Carlo Simulations using Neural Network Wave Function Ansatz *2019 - Present*

Project Lead, Lead Developer

https://github.com/NLESC-JCER/QMCTorch

**Votca XTP** GW-BSE for Excited States Quantum Chemistry *2019-Present*

Contributor : Matrix-free eigenvalue solvers on GPUs for large scale calculations

https://github.com/votca/xtp

**SWAN** Screening Workflows And Nanomaterials *2020-Present*

Contributor : Code Design

https://github.com/nlesc-nano/swan

**DeepRank** Deep learning framework for data mining protein-protein interactions *2017-Present*

Lead Developer

https://github.com/DeepRank/DeepRank

https://github.com/DeepRank/DeepRank-GNN

**iScore** support vector machines using random walk graph kernel for Protein-Protein Interaction *2019-Present*

Lead Developer

https://github.com/DeepRank/iscore

**pdb2sql** Fast and versatile biomolecular structure PDB file parser using SQL queries *2018-Present*

Lead Developer

https://github.com/DeepRank/pdb2sql

**Husky** Quantum Transport for Molecular Junctions *2017*

Lead Developer

https://github.com/nicorenaud/husky

## Closed Source Packages

**CHAMP** Quantum Monte Carlo Simulations of atomic and molecular systems *2018-Present*

Contributor : Code refactoring, Eigenvalue solvers

https://www.utwente.nl/en/tnw/ccp/research/CHAMP.html

**ADF** Amsterdam Density Functional *2017*

Contributor : Real-Time Time Dependent Density Functional Module

https://www.scm.com/

**TransPULL** Molecular Dynamics and quantum transport of single molecules *2014*

Contributor : Quantum transport

https://nanohub.org/resources/transpull

## Scientific Publications

2021 **DeepRank: A deep learning framework for data mining 3D protein-protein interfaces**
*Nicolas Renaud, Cunliang Geng, Sonja Georgievska, Francesco Ambrosetti, Lars Ridder, Dario F Marzella, Alexandre Bonvin, Li C Xue*
Nature Communication, Accepted for publication

2020 **Laserchicken—A tool for distributed feature calculation from massive LiDAR point cloud datasets**
*Christiaan Meijer, Meiert W. Grootes, Zsófia Koma, Yifat Dzigan, Romulo Gonçalves, Bouwe Andela, Gijs van den Oord, Elena Ranguelova, Nicolas Renaud, W. Daniel Kissling*
SoftwareX, vol. 12, 10026

2020 **The pdb2sql Python Package: Parsing, Manipulation and Analysis of PDB Files Using SQL Queries**
*Nicolas Renaud, Cunliang Geng*
Journal of Open Source Software, vol. 5, issue 49, pages 2077

2020 **Excited-state electronic structure of molecules using many-body Green's functions: Quasiparticles and electron–hole excitations with VOTCA-XTP**
*Gianluca Tirimbo, Vivek Sundram, Onur Caylak, Wouter Scharpach, Javier Sijen, Christoph Junghans, Joshua Brown, F Zapata Ruiz, Nicolas Renaud, Jens Wehner, Björn Baumeier*
The Journal of Chemical Physics, vol. 152, issue 11, pages 114103

2020 **iScore: An MPI supported software for ranking protein–protein docking models based on a random walk graph kernel and support vector machines**
*Nicolas Renaud, Yong Jung, Vasant Honavar, Cunliang Geng, Alexandre MJJ Bonvin, Li C Xue*
SoftwareX. vol. 11, pages 100462

2020 **iScore: a novel graph kernel-based function for scoring protein–protein docking models**
*Cunliang Geng, Yong Jung, Nicolas Renaud, Vasant Honavar, Alexandre MJJ Bonvin, Li C Xue*
Bioinformatics, vol. 36, issue 1, pages 112-121

2019 **Locating and controlling the Zn content in In (Zn) P quantum dots**
*Nicholas Kirkwood, Annick De Backer, Thomas Altantzis, Naomi Winckelmans, Alessandro Longo, Felipe V Antolinez, Freddy T Rabouw, Luca De Trizio, Jaco J Geuchies, Jence T Mulder, Nicolas Renaud, Sara Bals, Liberato Manna, Arjan J Houtepen*
Chemistry of Materials, vol. 32, issue 1, pages 557-565

2019 **The effect of the magnitude and direction of the dipoles of organic cations on the electronic structure of hybrid halide perovskites**
*Sudeep Maheshwari, Sameer Patwardhan, George C Schatz, Nicolas Renaud, Ferdinand C Grozema*
Physical Chemsitry Chemical Physics, vol. 21, issue 30, pages 16564-16572

2018 **Computational design of two-dimensional perovskites with functional organic cations**
*Sudeep Maheshwari, Tom J Savenije, Nicolas Renaud, Ferdinand C Grozema*
The Journal of Physical Chemistry C, vol. 122, issue 30, pages 17118-17122

2018 **Hot-electron transfer in quantum-dot heterojunction films**
*Gianluca Grimaldi, Ryan W Crisp, Stephanie Ten Brinck, Felipe Zapata, Michiko Van Ouwendorp, Nicolas Renaud, Nicholas Kirkwood, Wiel H Evers, Sachin Kinge, Ivan Infante, Laurens DA Siebbeles, Arjan J Houtepen*
Nature Communication, vol.9, issue 1, pages 1-10

2018 **Signatures of Conformational Dynamics and Electrode-Molecule Interactions in the Conductance Profile During Pulling of Single-Molecule Junctions**
*Leopoldo Mejía, Nicolas Renaud, Ignacio Franco*
The Journal of Physical Chemistry Letter, vol. 9, issue 4, pages 745-750

2017 **Interconversion between free charges and bound excitons in 2D hybrid lead halide perovskites**
*Maria C Gelvez-Rueda, Eline M Hutter, Duyen H Cao, Nicolas Renaud, Constantinos C Stoumpos, Joseph T Hupp, Tom J Savenije, Mercouri G Kanatzidis, Ferdinand C Grozema*
The Journal of Physical Chemistry C, vol. 121, issue 47. pages 26566-26574

2017 **Temperature dependent charge carrier dynamics in formamidinium lead iodide perovskite**
*María C Gélvez-Rueda, Nicolas Renaud, Ferdinand C Grozema*
The Journal of Physical Chemistry C, vol. 121, issue 42, pages 23392-23397

2017 **Design and characterization of an electrically powered single molecule on gold**
*Rémy Pawlak, Tobias Meier, Nicolas Renaud, Marcin Kisiel, Antoine Hinaut, Thilo Glatzel, Delphine Sordes, Corentin Durand, We-Hyo Soe, Alexis Baratoff, Christian Joachim, Catherine E Housecroft, Edwin C Constable, Ernst Meyer*
ACS Nano, vol. 11, issue 10, pages 9930-9940

2017 **Ga for Zn cation exchange allows for highly luminescent and photostable InZnP-based quantum dots**
*Francesca Pietra, Nicholas Kirkwood, Luca De Trizio, Anne W Hoekstra, Lennart Kleibergen, Nicolas Renaud, Rolf Koole, Patrick Baesjou, Liberato Manna, Arjan J Houtepen*
Chemistry of Materials, vol. 29, issue 12, pages 5192-5199

2017 **High electronic conductance through double-helix DNA molecules with fullerene anchoring groups**
*Kathia L Jiménez-Monroy, Nicolas Renaud, Jeroen Drijkoningen, David Cortens, Koen Schouteden, Christian Van Haesendonck, Wanda J Guedens, Jean V Manca, Laurens DA Siebbeles, Ferdinand C Grozema, Patrick H Wagner*
The Journal of Physical Chemistry A, vol. 121, issue 6, pages 1182-1188

2016 **Mechanically controlled quantum interference in individual π-stacked dimers**
*Riccardo Frisenda, Vera AEC Janssen, Ferdinand C Grozema, Herre SJ van der Zant, Nicolas Renaud*
Nature Chemistry - Cover Article, vol. 8, issue 12, pages 1099

2016 **Deep-hole transfer leads to ultrafast charge migration in DNA hairpins**
*Nicolas Renaud, Michelle A Harris, Arunoday PN Singh, Yuri A Berlin, Mark A Ratner, Michael R Wasielewski, Frederick D Lewis, Ferdinand C Grozema*
Nature Chemistry, vol. 8, issue 11, pages 1015-1021

2016 **Photogeneration and mobility of charge carriers in atomically thin colloidal InSe nanosheets probed by ultrafast terahertz spectroscopy**
*Jannika Lauth, Aditya Kulkarni, Frank CM Spoor, Nicolas Renaud, Ferdinand C Grozema, Arjan J Houtepen, Juleon M Schins, Sachin Kinge, Laurens DA Siebbeles*
The Journal of Physical Chemistry Letters, vol. 7, issue 20, pages 4191-4196

2016 **Effect of cation rotation on charge dynamics in hybrid lead halide perovskites**
*María C Gélvez-Rueda, Duyen H Cao, Sameer Patwardhan, Nicolas Renaud, Constantinos C Stoumpos, George C Schatz, Joseph T Hupp, Omar K Farha, Tom J Savenije, Mercouri G Kanatzidis, Ferdinand C Grozema*
The Journal of Physical Chemistry C, vol. 120, issue 30, pages 16577-16585

2016 **Tuning the Lattice Parameter of $In_xZn_yP$ for Highly Luminescent Lattice-Matched Core/Shell Quantum Dots**
*Francesca Pietra, Luca De Trizio, Anne W Hoekstra, Nicolas Renaud, Mirko Prato, Ferdinand C Grozema, Patrick J Baesjou, Rolf Koole, Liberato Manna, Arjan J Houtepen*
ACS Nano, vol. 10, issue 4,

2016 **Hole cooling is much faster than electron cooling in PbSe quantum dots**
*Frank CM Spoor, Lucas T Kunneman, Wiel H Evers, Nicolas Renaud, Ferdinand C Grozema, Arjan J Houtepen, Laurens DA Siebbeles*
ACS Nano, vol. 10, issue 1, pages 695-703

2016 **Computational design of donor-bridge-acceptor systems exhibiting pronounced quantum interference effects**
*Natalie Gorczak, Nicolas Renaud, Elena Galan, Rienk Eelkema, Laurens DA Siebbeles, Ferdinand C Grozema*
Physical Chemistry Chemical Physics, vol. 18, issue 9, pages 6773-6779

2015 **Conformationally gated charge transfer in DNA three-way junctions**
*Yuqi Zhang, Ryan M Young, Arun K Thazhathveetil, Arunoday PN Singh, Chaoren Liu, Yuri A Berlin, Ferdinand C Grozema, Frederick D Lewis, Mark A Ratner, Nicolas Renaud, Khatcharin Siriwong, Alexander A Voityuk, Michael R Wasielewski, David N Beratan*
The journal of physical chemistry letters, vol. 6, issue 13, pages 2434-2438

2015 **Charge transport across DNA-based three-way junctions**
*Ryan M Young, Arunoday PN Singh, Arun K Thazhathveetil, Vincent Y Cho, Yuqi Zhang, Nicolas Renaud, Ferdinand C Grozema, David N Beratan, Mark A Ratner, George C Schatz, Yuri A Berlin, Frederick D Lewis, Michael R Wasielewski*
Journal of the American Chemical Society, vol. 137, issue 15, pages 5113-5122

2015 **Intermolecular vibrational modes speed up singlet fission in perylenediimide crystals**
*Nicolas Renaud, Ferdinand C Grozema*
The journal of physical chemistry letters, vol. 6, issue 3, pages 360-365

2015 **Charge transfer versus molecular conductance: molecular orbital symmetry turns quantum interference rules upside down**
*Natalie Gorczak, Nicolas Renaud, Simge Tarkuç, Arjan J Houtepen, Rienk Eelkema, Laurens DA Siebbeles, Ferdinand C Grozema*
Chemical science, vol. 6, issue 7, pages 4196-4206

2014 **Cooperative biexciton generation and destructive interference in coupled quantum dots using adiabatic rapid passage**
*Nicolas Renaud, Ferdinand C Grozema*
Phys. Rev. B, vol. 90, issue 16, pages 165307

2014 **Large negative differential conductance in single-molecule break junctions**
*Mickael L Perrin, Riccardo Frisenda, Max Koole, Johannes S Seldenthuis, Jose A Celis Gil, Hennie Valkenier, Jan C Hummelen, Nicolas Renaud, Ferdinand C Grozema, Joseph M Thijssen, Diana Dulić, Herre SJ Van Der Zant*
Nature Nanotechnology vol. 9, issue 1, pages 830

2014 **Theoretical investigation of singlet fission in molecular dimers: The role of charge transfer states and quantum interference**
*Fatemeh Mirjani, Nicolas Renaud, Natalie Gorczak, Ferdinand C Grozema*
The journal of physical chemistry C vol. 118, issue 26, pages 14192-14199

2014 **Different mechanisms for hole and electron transfer along identical molecular bridges: the importance of the initial state delocalization**
*Natalie Gorczak, Simge Tarkuç, Nicolas Renaud, Arjan J Houtepen, Rienk Eelkema, Laurens DA Siebbeles, Ferdinand C Grozema*
The journal of physical chemistry A vol. 118, issue 22, pages 3891-3898

2014 **Impact of a single base pair substitution on the charge transfer rate along short DNA hairpins**
*Nicolas Renaud, Yuri A Berlin, Mark A Ratner*
Proceedings of the National Academy of Sciences vol. 110, issue 37, pages 14867-14871

2013 **Quantum interferences and electron transfer in photosystem I**
*Nicolas Renaud, Daniel Powell, Mahdi Zarea, Bijan Movaghar, Michael R Wasielewski, Mark A Ratner*
The Journal of Physical Chemistry A vol. 117, issue 29, pages 5899-5908

2013 **Mapping the relation between stacking geometries and singlet fission yield in a class of organic crystals**
*Nicolas Renaud, Paul A Sherratt, Mark A Ratner*
The journal of physical chemistry letters vol. 4, issue 7, pages 1065-1069

2013 **Between superexchange and hopping: An intermediate charge-transfer mechanism in poly (A)-poly (T) DNA hairpins**
*Nicolas Renaud, Yuri A Berlin, Frederick D Lewis, Mark A Ratner*
Journal of the American Chemical Society vol. 135, issue 10, pages 3953-3963

2013 **Decoherence and quantum interference in a four-site model system: Mechanisms and turnovers**
*Mahdi Zarea, Daniel Powell, Nicolas Renaud, Michael R Wasielewski, Mark A Ratner*
The Journal of Physical Chemistry B vol. 117, issue 4, pages 1010-1020

2013 **Decoherence and quantum interference in a four-site model system: Mechanisms and turnovers**
*Mahdi Zarea, Daniel Powell, Nicolas Renaud, Michael R Wasielewski, Mark A Ratner*
The Journal of Physical Chemistry B vol. 117, issue 4, pages 1010-1020

2013 **π-Dimerization of viologen subunits around the core of $C_60$ from twelve to six directions**
*Julien Iehl, Marco Frasconi, Henri-Pierre Jacquot de Rouville, Nicolas Renaud, Scott M Dyar, Nathan L Strutt, Ranaan Carmieli, Michael R Wasielewski, Mark A Ratner, Jean-François Nierengarten, J Fraser Stoddart*
Chemical Science vol. 4, issue 4, pages 1462-1469

2013 **π-Dimerization of viologen subunits around the core of $C_60$ from twelve to six directions**
*Julien Iehl, Marco Frasconi, Henri-Pierre Jacquot de Rouville, Nicolas Renaud, Scott M Dyar, Nathan L Strutt, Ranaan Carmieli, Michael R Wasielewski, Mark A Ratner, Jean-François Nierengarten, J Fraser Stoddart*
Chemical Science vol. 4, issue 4, pages 1462-1469

2013 **Binary Full-Adder in a Single Quantum System**
*Nicolas Renaud, Christian Joachim*
Architecture and Design of Molecule Logic Gates and Atom Circuits, 221-234

2012 **The different designs of molecule logic gates**
*Christian Joachim, Nicolas Renaud, Mohamed Hliwa*
Advanced Materials vol. 24, issue 2, pages 312-317

2011 **A stochastic surrogate Hamiltonian approach of coherent and incoherent exciton transport in the FMO complex**
*Nicolas Renaud, Mark A Ratner, Vladimiro Mujica*
The Journal of chemical physics vol. 135, issue 7, pages 08B617

2011 **A time-dependent approach to electronic transmission in model molecular junctions**
*Nicolas Renaud, Mark A Ratner, Christian Joachim*
The Journal of Physical Chemistry B vol. 115, issue 18, pages 5582-5592

2011 **Demonstration of a NOR logic gate using a single molecule and two surface gold atoms to encode the logical input**
*W-H Soe, C Manzano, A De Sarkar, F Ample, N Chandrasekhar, N Renaud, P de Mendoza, AM Echavarren, M Hliwa, C Joachim*
Physical Review B vol. 83, issue 15, pages 155443

2011 **Classical Boolean logic gates with quantum systems**
*Nicolas Renaud, Christian Joachim*
Journal of Physics A: Mathematical and Theoretical vol. 44, issue 15, pages 155302

2011 **Manipulating molecular quantum states with classical metal atom inputs: demonstration of a single molecule NOR logic gate**
*We-Hyo Soe, Carlos Manzano, Nicolas Renaud, Paula de Mendoza, Abir De Sarkar, Francisco Ample, Mohamed Hliwa, Antonio M Echavarren, Natarajan Chandrasekhar, Christian Joachim*
ACS Nano vol. 5, issue 2, pages 1436-1440

2011 **Single molecule logical devices**
*Nicolas Renaud, Mohamed Hliwa, Christian Joachim*
Unimolecular and Supramolecular Electronics II, pages 217-268

2009 **A NOR–AND quantum running gate molecule**
*Nicolas Renaud, Masa Ito, We-Hyo Shangguan, Mark Saeys, Mohamed Hliwa, Christian Joachim*
Chemical Physics Letter, vol 472, issue 1, page 74-79

2008 **Design and stability of NOR and NAND logic gates constructed with three quantum states**
*Nicolas Renaud, Christian Joachim*
Physical Review A, vol 78, issue 6, page 062316

2008 **An intramolecular digital 1/2-adder with tunneling current drive and read-outs**
*Ivan Duchemin, Nicolas Renaud, Christian Joachim*
Chemical Physics Letters, vol 452, issue 4, page 269-274