

Deniz Tuna

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Postdoctoral Research Experience

- 05/2017–present **Stanford University**, Stanford, USA and **SLAC National Accelerator Laboratory**, Menlo Park, USA
Advisor: Todd J. Martínez.
Research focus: Ab initio multiple spawning nonadiabatic dynamics simulations of biochromophores in solution and in protein environments with QM/MM.
- 05/2014–04/2017 **Max-Planck-Institut für Kohlenforschung**, Mülheim an der Ruhr, Germany
Advisor: Walter Thiel.
Research focus: Application of semiempirical methods to electronically excited states of organic and biomolecules. Benchmarks of linear-response and semiempirical methods for excited states and conical intersections. Trajectory-surface-hopping nonadiabatic dynamics simulations of biomolecules.

Education

- 04/2014 **Technische Universität München**, Garching, Germany: conferment of *Dr. rer. nat.* degree. Grade: *summa cum laude* (“with highest distinction”).
- 01/2010–04/2014 **Technische Universität München**, Garching, Germany: doctoral student. Advisor: Wolfgang Domcke. Title of thesis: “Quantum-Chemical

Investigations into the Photophysics and Photochemistry of Bioorganic Molecules”.

- 12/2009 **Philipps-Universität Marburg**, Marburg, Germany: conferment of “*Diplom-Chemiker*” degree. Grade: 1.1 (on a scale from 1.0 to 5.0 with 1.0 being the best possible grade).
- 03/2009–12/2009 **Technische Universität München**, Garching, Germany: research for diploma thesis. Advisor: Wolfgang Domcke. First examiner at Philipps-Universität Marburg: Gernot Frenking.
- 10/2007–03/2008 **Heriot-Watt University**, Edinburgh, Scotland, UK: study-abroad semester. Research project (six months) in computational chemistry. Supervisor: Stuart A. Macgregor. Resulted in publication no. 1.
- 04/2006–02/2009 **Philipps-Universität Marburg**, Marburg, Germany: main-study period in Chemistry. Elective subject of specialization: Theoretical Chemistry.
- 04/2004–03/2006 **Heinrich-Heine-Universität Düsseldorf**, Düsseldorf, Germany: Basic-study period in Chemistry. Completed with “*Vordiplom*”. Grade: “*sehr gut*” / “very good” (on a scale from “very good” to “failed”).

Awards, Grants and Fellowships

- 05/2017–present Research Fellowship (82,599 EUR) from Deutsche Forschungsgemeinschaft (DFG) / German Research Foundation for a postdoctoral research appointment at Stanford University.
- 07/2013 Young Researcher, 63rd Lindau Nobel Laureate Meeting, Lindau, Germany. Selected as one of ~600 participants from thousands of applicants.
- 07/2013 Scholarship for participation in the 63rd Lindau Nobel Laureate Meeting, Lindau, Germany, from the National Academy of Science and Engineering (acatech) and *Verband der Chemischen Industrie e.V.*

- 08/2010–04/2014 Doctoral fellowship and 3-year stipend from the International Max-Planck Research School of Advanced Photon Science (IMPRS-APS) of the Max-Planck-Institut für Quantenoptik, Garching, Germany.
- 10/2007–03/2008 Scholarship from German Academic Exchange Services (DAAD) for a study-abroad semester at Heriot-Watt University, Edinburgh, Scotland.
- 03/2006–12/2009 Fellow of “Studienstiftung des deutschen Volkes” / “German Academic National Foundation”.

Research Interests

- since 2009 Photochemistry, photophysics and electronically excited states of organic and bioorganic molecules; quantum chemistry for electronically excited states; identification and description of conical intersections; nonadiabatic dynamics simulations of photoexcited molecules; QM/MM studies of photoactive proteins and solvated chromophores.

Publications

Peer-Reviewed Journal Articles

15. **Deniz Tuna**, Lasse Spörkel, Mario Barbatti and Walter Thiel: Nonadiabatic Dynamics Simulations of Photoexcited Urocanic Acid. *Chem. Phys.* **2018**, *515*, 521–534.
14. Daniel Lefrancois, **Deniz Tuna**, Todd J. Martínez and Andreas Dreuw: The Spin-Flip Variant of the Algebraic-Diagrammatic Construction Yields the Correct Topology of S_1/S_0 Conical Intersections. *J. Chem. Theory Comput.* **2017**, *13*, 4436–4441.
13. **Deniz Tuna**, Andrzej L. Sobolewski and Wolfgang Domcke: Conical-Intersection Topographies Suggest That Ribose Exhibits Enhanced UV Photostability. *J. Phys. Chem. B* **2016**, *120*, 10729–10735.

12. **Deniz Tuna**, You Lu, Axel Koslowski and Walter Thiel: Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks of Electronically Excited States. *J. Chem. Theory Comput.* **2016**, *12*, 4400–4422.
11. **Deniz Tuna**, Anikó Udvarhelyi, Andrzej L. Sobolewski, Wolfgang Domcke and Tatiana Domratcheva: Onset of the Electronic Absorption Spectra of Isolated and π -Stacked Oligomers of 5,6-Dihydroxyindole: An Ab Initio Study of the Building Blocks of Eumelanin. *J. Phys. Chem. B* **2016**, *120*, 3493–3502.
10. Pavlina Kancheva, **Deniz Tuna** and Vassil B. Delchev: Comparative study of radiationless deactivation mechanisms in cytosine and 2,4-diaminopyrimidine. *J. Photochem. Photobiol. A* **2016**, *321*, 266–274.
9. **Deniz Tuna** and Wolfgang Domcke: Excited-state deactivation in 8-oxo-deoxyguanosine: comparison between anionic and neutral forms. *Phys. Chem. Chem. Phys.* **2016**, *18*, 947–955.
8. **Deniz Tuna**, Daniel Lefrancois, Łukasz Wolański, Samer Gozem, Igor Schapiro, Tadeusz Andruniów, Andreas Dreuw and Massimo Olivucci: Assessment of Approximate Coupled-Cluster and Algebraic-Diagrammatic-Construction Methods for Ground- and Excited-State Reaction Paths and the Conical-Intersection Seam of a Retinal-Chromophore Model. *J. Chem. Theory Comput.* **2015**, *11*, 5758–5781.
7. Tolga N. V. Karsili, **Deniz Tuna**, Johannes Ehrmaier and Wolfgang Domcke: Photoinduced water splitting via benzoquinone and semiquinone sensitisation. *Phys. Chem. Chem. Phys.* **2015**, *17*, 32183–32193.
6. **Deniz Tuna**, Nađa Došlić, Momir Mališ, Andrzej L. Sobolewski and Wolfgang Domcke: Mechanisms of Photostability in Kynurenines: A Joint Electronic-Structure and Dynamics Study. *J. Phys. Chem. B* **2015**, *119*, 2112–2124.
5. **Deniz Tuna**, Andrzej L. Sobolewski and Wolfgang Domcke: Photochemical Mechanisms of Radiationless Deactivation Processes in Urocanic Acid. *J. Phys. Chem. B* **2014**, *118*, 976–985.

4. **Deniz Tuna**, Andrzej L. Sobolewski and Wolfgang Domcke: Mechanisms of Ultrafast Excited-State Deactivation in Adenosine. *J. Phys. Chem. A* **2014**, *118*, 122–127.
3. **Deniz Tuna**, Andrzej L. Sobolewski and Wolfgang Domcke: Electronically excited states and photochemical reaction mechanisms of β -glucose. *Phys. Chem. Chem. Phys.* **2014**, *16*, 38–47. (Featured on the cover of issue 1.)
2. Rafał Szabla, **Deniz Tuna**, Robert W. Góra, Jiří Šponer, Andrzej L. Sobolewski and Wolfgang Domcke: Photochemistry of 2-Aminooxazole, a Hypothetical Prebiotic Precursor of RNA Nucleotides. *J. Phys. Chem. Lett.* **2013**, *4*, 2785–2788.
1. Torstein Fjermestad, Joanne H. H. Ho, Stuart A. Macgregor, Barbara A. Messerle and **Deniz Tuna**: Computational Study of the Mechanism of Cyclic Acetal Formation via the Iridium(I)-Catalyzed Double Hydroalkoxylation of 4-Pentyn-1-ol with Methanol. *Organometallics* **2011**, *30*, 618–626.

Invited Seminar Talks

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| 04/2017 | In the group of Wolfgang Domcke, Technische Universität München, Garching, Germany. |
| 01/2015 | In the group of Christel M. Marian, Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany. |
| 03/2014 | In the group of Walter Thiel, Max-Planck-Institut für Kohlenforschung, Mülheim, Germany. |
| 08/2011 | In the group of Tatiana Domratcheva, Max-Planck-Institut für Medizinische Forschung, Department of Biomolecular Mechanisms, Heidelberg, Germany. |

Conference Participation and Contributions

- 03/2018 West Coast Theoretical Chemistry Symposium, Stanford, USA. *Poster presentation.*
- 08/2017 11th World Congress of the World Association of Theoretical and Computational Chemists (WATOC), Munich, Germany. *Poster presentation.*
- 06/2016 8th Molecular Quantum Mechanics (MQM), Uppsala, Sweden. *Poster presentation.*
- 09/2015 51st Symposium für Theoretische Chemie, Potsdam, Germany. *Contributed talk.*
- 04/2015 “Modeling Photoactive Molecules”, Nantes, France (organized by Prof. Denis Jacquemin and Dr. Adèle Laurent). *Contributed talk.*
- 10/2014 10th World Congress of the World Association of Theoretical and Computational Chemists (WATOC), Santiago, Chile. *Poster presentation.*
- 09/2014 50th Symposium für Theoretische Chemie, Vienna, Austria. *Poster presentation.*
- 07/2013 63rd Lindau Nobel Laureate Meeting on Chemistry, Lindau, Germany.
- 08/2012 244th ACS National Meeting, Philadelphia, Pennsylvania, USA. *Poster presentation.*
- 06/2012 14th International Congress on Quantum Chemistry, Boulder, Colorado, USA and its satellite symposium “Advances in Quantum Chemistry: Interfacing Electronic Structure with Dynamics”, Minneapolis, Minnesota, USA. *Poster presentations.*
- 03/2012 243rd ACS National Meeting, San Diego, California, USA. *Two contributed talks.*
- 07/2011 9th World Congress of the World Association of Theoretical and Computational Chemists (WATOC), Santiago de Compostella, Spain, and

its satellite meeting “Excited states and non-adiabatic processes in complex systems”, St. Feliu de Guíxols, Spain. *Poster presentations*.

02/2011 Workshop on Theoretical Chemistry: “Explicitly Correlated Methods”, Mariapfarr, Austria.

09/2010 46th Symposium für Theoretische Chemie, Münster, Germany. *Poster presentation*.

Research Visits

2010–2012 Four weeks in total in the group of Andrzej L. Sobolewski, Institute of Physics, Polish Academy of Science, Warsaw, Poland. Resulted in several joint publications.

10/2011 One day in the group of Mario Barbatti, Max-Planck-Institut für Kohlenforschung, Mülheim, Germany. Resulted in publication no. 15.

08/2011 One week in the group of Tatiana Domratcheva, Max-Planck-Institut für Medizinische Forschung, Department of Biomolecular Mechanisms, Heidelberg, Germany. Resulted in publication no. 11.

Supervision of Research / Mentoring and Advising

04/2016–04/2017 Hendrik H. Heenen, visiting PhD student of Karsten Reuter, Technische Universität München, and external collaborator. Joint publication in preparation.

03/2014 Johannes Ehrmaier, non-mandatory research project during master’s studies (one month). Resulted in publication no. 7.

03/2013 Rafał Szabla, visiting PhD student of Jiří Šponer, Institute of Biophysics, Academy of Sciences of the Czech Republic, Brno, Czech Republic (one month). Resulted in publication no. 2.

09/2012–10/2012 Pavlina Kancheva, visiting PhD student of Vassil B. Delchev, University of Plovdiv, Bulgaria (two months). Resulted in publication no. 10.

- 09/2011–10/2011 Hendrik H. Heenen, mandatory research project for master's degree (six weeks). Joint publication in preparation (see above).
- 10/2011–08/2012 Rafał Szabla, master's thesis (nine months). Resulted in publication no. 2.
- 03/2011–05/2011 Hendrik H. Heenen, bachelor's thesis (two months).

Teaching Experience

- 10/2013 Teaching assistant of Karsten Reuter, Ulrich K. Heiz, Thomas Kiefhaber, Hubert Gasteiger, Technische Universität München, for the course "Measurement, Analysis & Simulation". Two four-hour tutorial sessions on basic programming in MATLAB (20 students).
- 2010–2013 Presentation on computational chemistry and its applications to 2nd-year B.Sc. students of Quantum Mechanics (one hour).
- 10/2012–04/2013 Head teaching assistant of Wolfgang Domcke, Technische Universität München, for the lecture "Introduction to Quantum Mechanics and Group Theory". Design of 14 two-hour tutorial lessons (81 assignments in total), stand-in lecturer on two occasions, design and grading of two written exams (12 assignments each, taken by 127 and 31 examinees).
- 04/2009–09/2012 Teaching assistant of Wolfgang Domcke, Karsten Reuter, Notker Rösch, Mathias Nest, Christoph Scheurer, Technische Universität München. Teaching of tutorial lessons for the lectures "Introduction to Quantum Mechanics and Group Theory", "Computational Chemistry", "Molecular Modelling", and "Mathematical Methods in Chemistry". 15 two-hour tutorial lessons (~30 students per course) and grading of two written exams (taken by 30 to 150 examinees) per semester.
- 10/2006–02/2007 Teaching assistant of Bernhard Roling, Philipps-Universität Marburg. Teaching of tutorial lessons for the lecture "Physical Chemistry 0". 15 two-hour tutorial lessons (25 students) and grading of one written exam (taken by 60 examinees).
- 10/2005–02/2006 Teaching assistant of Timo Fleig, Institute of Theoretical and Computational Chemistry, Heinrich-Heine Universität Düsseldorf.

Teaching of tutorial lessons for the lecture “Theoretical Chemistry I”. 10 two-hour tutorial lessons (20 students).

Professional Service

- since 2012 Peer-review of 20 manuscripts for the journals *The Journal of Physical Chemistry Letters*, *The Journal of Physical Chemistry*, *PCCP*, *Chemical Physics*, *ChemPhysChem*, *Photochemistry and Photobiology*, *International Journal of Molecular Sciences*, *Chemistry - A European Journal*, *RSC Advances* and *Journal of Raman Spectroscopy*.
- 05/2010–03/2013 Nomination of three B.Sc. students by letter of recommendation for a fellowship from “Studienstiftung des deutschen Volkes” / “German Academic National Foundation”.

Workshops, Seminars, Summer Schools and Contributions

- 09/2018 18th Annual German Academic International Network (GAIN) Conference, Boston, USA (two days).
- 03/2018 TeraChem/FMS Developers’ Workshop, Stanford, USA (two days). *Oral presentation*.
- 08/2017–03/2018 Attendance of 5 seminars on the academic job search and application process, Stanford Career Education, Stanford, USA.
- 2014–2017 Attendance of ~30 scientific seminar and colloquium talks at Max-Planck-Institut für Kohlenforschung, Max-Planck-Institut for Chemical Energy Conversion, University of Duisburg-Essen, University of Düsseldorf and Ruhr-Universität Bochum.
- 2009–2014 Attendance of ~50 scientific seminar and colloquium talks at Technische Universität München, Ludwig-Maximilians-Universität München, Max-Planck-Institute for Quantum Optics and Institute of Physics of the Polish Academy of Sciences.

- 11/2013 IMPRS-APS Annual Meeting (one day), Nicholas Karpovicz, Vlad Yakovlev, Kreuth, Germany. *Oral presentation.*
- 07/2012 IMPRS-APS Annual Meeting (two days), Nicholas Karpovicz, Vlad Yakovlev, Kreuth, Germany. *Oral presentation.*
- 03/2012 Final seminar of TUM Graduate School (one day), Garching, Germany.
- 02/2012 “Scientific Proposal Writing” (one day), Bodil Holst, Munich, Germany.
- 11/2011 Kick-Off Seminar “Be Interdisciplinary” of TUM Graduate School (three days), Herrsching, Germany.
- 06/2011 Introduction to NWChem (one day), Karol Kowalski, Tjerk P. Straatsma, Garching, Germany.
- 04/2011 “Scientific Paper Writing” (one day), Bodil Holst, Munich, Germany, and “Scientific Writing” (two days), Elisabeth Grenzebach, Garching, Germany.
- 12/2010 IMPRS-APS Annual Meeting (one day), Peter Hommelhoff, Munich, Germany. *Oral presentation.*
- 11/2010 IMPRS Interdisciplinary Symposium “New Frontiers in Science” (two days), Munich, Germany.
- 08/2010 IMPRS Summer School (four days), Wildbad Kreuth, Germany. *Poster presentation.*
- 05/2010 IMPRS Candidates Selection Round (one day), Garching, Germany. *Oral presentation.*
- 08/2008 Summer School of Studienstiftung des deutschen Volkes (two weeks), Neubeuern, Germany. Seminar on “Faszination Mathematik” (“Fascination Mathematics”) by Rainer Löwen and Harald Löwe. *Oral presentation* on “The Pigeonhole Principle”.
- 09/2007 Summer School of Studienstiftung des deutschen Volkes (two weeks), Görlitz, Germany. Seminar on “Moderne Quantensysteme” (“Modern

Quantum Systems”) by Christoph Bruder and Florian Marquardt. *Oral presentation* on “The Fundamentals of Quantum Computing”.

09/2006 Language Course at Hilderstone College (three weeks), Broadstairs, England, UK. Certified CETR level: C2 (“Mastery”).

Languages

German Mother tongue

English Proficient

Professional Memberships or Affiliations

since 2014 American Chemical Society (ACS)

since 2004 Gesellschaft Deutscher Chemiker (GDCh)