Johannes Tölle | Curriculum Vitae

Friedrich-Ebert-Straße 177 – 48153 Münster – Germany

+49 (157) 796 77990 • j_toel01@wwu.de

Personal Details

Date of Birth: 15.02.1995

Place of Birth: Düsseldorf

Citizenship: German

Civil status: Single

Education

Westfälische Wilhelms-Universität — **Münster**
Postdoc — *September 2021 -*

Westfälische Wilhelms-Universität — **Münster**
PhD, Grade: summa cum laude (with distinction) — *1.10.2018–02.09.2021*
Subsystem-Based Modeling of Photo-Induced Processes

Rutgers University — **Newark, USA**
Research Stay — *04.08.2017–10.02.2018*
with M. Pavanello (theoretical chemistry)

Westfälische Wilhelms-Universität — **Münster**
Master of Science, Grade: 1.1 (very good) — *2016–2018*
Focus on spectroscopy, organic- and theoretical chemistry

Westfälische Wilhelms-Universität — **Münster**
Bachelor of Science, Grade: 1.9 (good) — *2013–2016*
General chemistry

Konrad-Heresbach-Gymnasium — **Mettmann**
General higher education entrance qualification (Abitur), Grade: 1.6 — *2005–2013*

Bachelor Thesis

Title: *Adaptive QM/MM on Graphical Processing Units*

Supervisors: PD Dr. Mark Waller, Prof. Dr. Johannes Neugebauer

Grade: 1.0 (very good)

Master Thesis

Title: *Time Dependent Density Functional Theory with reduced orbital space*

Supervisor: Prof. Dr. Johannes Neugebauer

Grade: 1.0 (very good)

Doctoral Thesis

Title: *Subsystem-Based Modeling of Photo-Induced Processes*

Supervisor: Prof. Dr. Johannes Neugebauer

Grade: summa cum laude (with distinction)

Further education

Molecular Response Properties Winterschool — **Haraldvollen, Norway**
Organizers: K. Ruud, P. Norman, T. Saue — *14.01.2019–18.01.2019*
Lecturer: K. Ruud, P. Norman, T. Saue

European Summerschool in Quantum Chemistry (ESQC) — **Sicily, Italy**
Organizer: T. Saue — *08.09.2019–21.09.2019*
Lecturer: T. Saue, W. Klopper, D. Crawford, T. Helgakar, F. Manby, F. Neese, J. Olsen, J. Toulouse, P.O. Widmark, P. Taylor

Research Profile

Expertise

- Method development in the field of ground and excited state subsystem Density-Functional Theory for periodic and non-periodic systems
- Method development in the field of subsystem GW and the Bethe–Salpeter-Equation
- Software development [Serenity, embedded Quantum Espresso (eQE)]
- Machine Learning and Data Science [Data Science Lecture by Patrick Shafto at Rutgers University Newark; Co-organized hands-on-session on molecular mashine learning, Organic-Chemistry Institute University of Münster]

Collaboration

- Prof. Dr. Michele Pavanello (Rutgers University, Newark)
- Prof. Dr. Benedetta Mennucci, Prof. Dr. Lorenzo Cupellini (University of Pisa)
- Prof. Dr. Michael Rohlfing, Dr. Thorsten Deilmann (University of Münster)

Theses Co-Supervised

- 2019: Bachelor Thesis: "Implementation and application of simplified Tamm–Dancoff Density-Functional Theory", Lukas Paetow
- 2019: Master Thesis: "Solvents Effects on Response Properties in Subsystem Time-Dependent Density-Functional Theory", Niklas Niemeyer
- 2020: Master Thesis: "Bridging the gap between molecular and periodic approaches in subsystem Density-Functional Theory", Lukas Paetow
- 2020: Bachelor Thesis: "Implementierung und Anwendung von Methoden zur Analyse elektronischer Anregungen in Molekülen", Anton Rikus

Publications

1. **J. Tölle** T. Deilmann, M. Rohlfing, J. Neugebauer, 'Subsystem-based GW/Bethe–Salpeter-Equation', *J. Chem. Theory Comput.*, **2021**, 17, 2186
2. **J. Tölle**, L. Cupellini, B. Mennucci, J. Neugebauer, 'Electronic Couplings for Photo-Induced Processes from Subsystem Time-Dependent Density-Functional Theory: The Role of the Diabati-

zation', *J. Chem. Phys.*, **2020**, 153, 184113

3. N. Niemeyer, **J. Tölle**, J. Neugebauer, 'Approximate versus Exact Embedding for Chiroptical Properties: Reconsidering Failures in Potential and Response', *J. Chem. Theory Comput.*, **2020**, 16, 3104
4. L. Scholz, **J. Tölle**, J. Neugebauer, 'Analysis of Environment Response Effects on Excitation Energies within Subsystem-based Time-Dependent Density-Functional Theory', *Int. J. Quantum Chem.*, **2020**, e26213
5. **J. Tölle**, M. Böckers, N. Niemeyer, J. Neugebauer, 'Inter-Subsystem Charge-Transfer Excitations in Exact Subsystem Time-Dependent Density-Functional Theory', *J. Chem. Phys*, **2019**, 151, 174109
6. **J. Tölle**, M. Böckers, J. Neugebauer ,'Exact Subsystem Time-Dependent Density-Functional Theory', *J. Chem. Phys*, **2019**, 150, 181101
7. **J. Tölle**, P. Ramos, A. S. P. Gomes, M. Pavanello, 'Charged-cell Periodic DFT Simulations Via an Impurtiy Model Based on Density Embedding: Application to the ionization potential of liquid water', *Int. J. of Quantum. Chem.*, **2019**, 119, e25801
   (top 10% of the most downloaded articles in the Int. J. of Quantum Chem. 2018 -2019)

Talks

16.05.2019: 'Exact Subsystem Time-Dependent Density-Functional Theory (sTDDFT)', *CMTC Mini-symposium on Uncertainty in Quantum Chemistry*, Münster, Germany

26.08.2019: 'Exact Subsystem Time-Dependent Density-Functional Theory (sTDDFT)', *Invited to group seminar*, Rutgers Newark, USA

24.09.2019: 'Exact Subsystem Time-Dependent Density-Functional Theory (sTDDFT)', *Symposium on theoretical chemistry (STC 2019)*, Rostock, Germany

12.11.2020: 'Subsystem Time-Dependent Density-Functional Theory for modeling of Photo-Induced Process', *Organic-Chemistry Institute's Colloquium*, Münster, Germany

01.04.2021: 'Subsystem-Based Modeling of Photo-Induced Processes', *Virtual group seminar, Chan Group*, California Institute of Technology, USA

Posters

06.11.2017: 'Cluster Embedding Theory based on periodic subsystem Density-Functional Theory', *High Performance Computing Fair*, Rutgers Newark, USA

06.06.2019: 'An Exact Quantum Chemical Fragmentation Method for Excited States', *FoChIn (Forschung der Chemischen Industrie)*, WWU Münster, Germany

16.09.2019: 'Exact Subsystem Time-Dependent Density-Functional Theory', *European Summer-school in Qunatum Chemistry (ESQC)*, Sicily, Italy

21.09.2021: 'Subsystem-Based GW/Bethe–Salpeter Equation', *Virtual Symposium on theoretical chemistry (STC 2021)*, Würzburg

08-11.11.2021: 'Subsystem-Based GW/Bethe–Salpeter Equation', *Computational Methods in Photosynthesis (ComPhot 2021)*, Virtual conference