

Dr. Matthias Degroote | CV

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in mfmdegroote

Education at Ghent University

PhD in Physics Center for Molecular Modeling Thesis title: Faddeev random phase approximation for molecules Supervisor: Dimitri Van Neck	2008–2012
MSE in Applied Physics Faculty of Engineering and Architecture	2006–2008
MS in Physics Faculty of Sciences Unfinished due to start of PhD in Physics	2006–2008
BS in Physics Faculty of Sciences	2005–2008
BSE in Applied Physics Faculty of Engineering and Architecture	2003–2006

Scientific Career

Postdoctoral Researcher Department of Chemistry, Rice University	2014–2017
Postdoctoral Researcher Department of Physics, Ghent University	2013–2014
Postdoctoral Researcher Center for Molecular Modeling, Ghent University	2012–2012

Grants and Fellowships

2017–present: PI of a start-up allocation from the National Science Foundation (NSF) Extreme Science and Engineering Discovery Environment (XSEDE)

2016–present: Postdoctoral Research Fellow of the Center for the Computational Design of Functional Layered Materials (CCDM)

2014–2015: Postdoctoral fellowship of the Belgian American Educational Foundation (BAEF)

2008–2012: PhD fellowship of the National Science Foundation of Flanders (FWO)

Research Experience

Coupled Cluster methods 2014–2017

Scuseria Group, Department of Chemistry, Rice University
Symmetry breaking and restoration. Development of the Polynomial Similarity Transform for the BCS hamiltonian. Gutzwiller Similarity Transform for the Hubbard model

Projected Entangled Pair States 2013–2014

Verstraete Group, Department of Physics, Ghent University
Development of the transfer matrix formalism for excited states of the 2D AKLT hamiltonian.

Green's Function theory 2008–2012

Center for Molecular Modeling, Ghent University
Excited states with combined particle-particle and particle-hole RPA for diatomic molecules.

Teaching Experience at the Center for Molecular Modeling

Molecular Structure 2011–2012

Teaching assistant for Michel Waroquier and Veronique Van Speybroeck.
Stand in for theory and regular exercise sessions.

Master Thesis Advisor 2011–2012

Daily guidance under the supervision of Dimitri Van Neck.
Topic: Matrix Product States

Master Thesis Advisor 2011–2012

Daily guidance under the supervision of Dimitri Van Neck.
Topic: DFT and Green's function methods

Master Thesis Advisor 2010–2011

Daily guidance under the supervision of Dimitri Van Neck.
Topic: Green's function methods

Quantum Mechanics I 2008–2012

Teaching assistant for Michel Waroquier.
Exercise sessions, student questions, making and grading exercise exam

Publications

- [1] J. A. Gomez, **M. Degroote**, J. Zhao, Y. Qiu, and G. E. Scuseria. Spin polynomial similarity transformation for repulsive hamiltonians: Interpolating between coupled cluster and spin-projected unrestricted hartree-fock. *Phys. Chem. Chem. Phys.*, pages –, 2017.
- [2] J. M. Wahlen-Strothman, T. M. Henderson, M. R. Hermes, **M. Degroote**, Y. Qiu, J. Zhao, J. Dukelsky, and G. E. Scuseria. Merging symmetry projection methods with coupled cluster theory: Lessons from the lipkin model hamiltonian. *The Journal of Chemical Physics*, 146(5):054110, Feb 2017.
- [3] **M. Degroote**, T. M. Henderson, J. Zhao, J. Dukelsky, and G. E. Scuseria. Polynomial similarity transformation theory: A smooth interpolation between coupled cluster doubles and projected BCS applied to the reduced BCS hamiltonian. *Phys. Rev. B*, 93:125124, Mar 2016.
- [4] V. Zauner, D. Draxler, L. Vanderstraeten, **M. Degroote**, J. Haegeman, M. M. Rams, V. Stojevic, N. Schuch, and F. Verstraete. Transfer matrices and excitations with matrix product states. *New Journal of Physics*, 17(5):053002, 2015.
- [5] **M. Degroote**. Faddeev random phase approximation applied to molecules. *The European Physical Journal Special Topics*, 218(1):1–70, 2013.
- [6] H. van Aggelen, B. Verstichel, G. Acke, **M. Degroote**, P. Bultinck, P. W. Ayers, and D. Van Neck. Extended random phase approximation method for atomic excitation energies from correlated and variationally optimized second-order density matrices. *Computational and Theoretical Chemistry*, 1003:50–54, Jan 2012.
- [7] C. Barbieri, D. Van Neck, and **M. Degroote**. Accuracy of the Faddeev random phase approximation for light atoms. *Physical Review A*, 85:012501, Jan 2012.
- [8] **M. Degroote**, D. Van Neck, and C. Barbieri. Faddeev random-phase approximation for molecules. *Physical Review A*, 83:042517, Apr 2011.
- [9] **M. Degroote**, D. Van Neck, and C. Barbieri. Faddeev random phase approximation for molecules. *Computer Physics Communications*, 182(9):1995 – 1998, 2011. Computer Physics Communications Special Edition for Conference on Computational Physics Trondheim, Norway, June 23-26, 2010.

Contributions at international conferences and meetings

2017: Contributed talk at the *254th American Chemical Society National Meeting & Exposition, Washington DC*

2017: Contributed talk at the *3rd Annual Smalley-Curl Institute Summer Research Colloquium, Houston*

2017: Invited seminar at the *Laboratoire de Chimie Théorique, Jussieu, France*

2017: Invited seminar at the *Smalley Curl Institute, Houston*

2017: Invited seminar at the *Center for Molecular Modeling, Ghent, Belgium*

2016: Poster at *Low-scaling and Unconventional Electronic Structure Techniques Conference, Telluride*

2014: Poster at *Low-scaling and Unconventional Electronic Structure Techniques Conference, Telluride*

2013: Poster at *7th Molecular Quantum Mechanics 2013, Lugano, Switzerland*

2012: Organizer and speaker at *Mini-workshop on Recent Developments in Green's Function Methods, Ghent, Belgium*

2012: Invited seminar at the *Institut de Physique Nucléaire d'Orsay, France*

2011: Poster at *International Conference on Recent Progress in Many-Body Theories (RPMBT16), Bariloche, Argentina*

2011: Poster at *The 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), Tokyo, Japan*

2011: Contributed talk at *Fermions from Cold Atoms to Neutron Stars: Benchmarking the Many-Body Problem (INT-11-1), Seattle*

2010: Contributed talk at *Conference on Computational Physics (CCP2010), Trondheim, Norway*

2010: Contributed talk at *ECT* workshop: Reactions and Nucleon Properties in Rare Isotopes, Trento, Italy*

Community Involvement and Outreach

2017: SCI Colloquium 2017

Poster judge at the 3rd Annual Summer Research Colloquium of the Smalley-Curl Institute.

2016–2017: PAIR Houston

College mentor program of the Partnership for the Advancement and Immersion of Refugees. Weekly meetings with a high school senior who came to the US through a resettlement program. Trying to be a guide and mentor in the process of enlisting in higher education and everything that is involved.

2017: APSS 2017

Abstract judge at the 7th MD Anderson Annual Postdoctoral Science Symposium.

2017: RURS 2017

Poster judge at the Rice Undergraduate Research Symposium for the School of Natural Sciences.

2011–2014: Uilenspel VZW

Weekly one on one homework mentoring for disadvantaged children ages 6-8 with learning problems. Bridging the gap with peers through highly tailored exercises and games.

2008–2014: Public schools career fairs

Talking about the academic world as a career choice to high school science classes. Short presentations followed by a Q&A session.