CURRICULUM VITAE - Henk Eshuis

Personal Information

Henk Eshuis
Montclair State University
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Appointments

- 2017-to date: Associate Professor of Chemistry at Montclair State University
- 2012-2017: Assistant Professor of Chemistry at Montclair State University

Academic Training and Qualifications

- 2009-2012: Postdoctoral research fellow at University of California, Irvine
- 2005-2009: PhD Chemistry at Bristol University, United Kingdom
- 2003-2005: Doctoraal diploma Chemistry, Cum Laude, Utrecht University, The Netherlands
- 1998-2000: Reading Theology, Utrecht University, The Netherlands
- 1996-1998: Propaedeuse Chemistry, Cum Laude, Utrecht University, The Netherlands

Other Education

- 2007: The Landmark Forum and Advanced Course from Landmark Education

Teaching Experience

- Physical Chemistry I and II and Experimental Physical Chemistry
- General Chemistry I and II, both lecture and laboratory
- 2012 and 2015: Graduate course in Computational Chemistry
- Summer 2011: Instructor for CHEM 5 Scientific Computing Skills
- 2007-2008: Tutoring Maths 1S tutorial to undergraduate students
- 2005-2007: Demonstrating Level 2 Theoretical Chemistry Workshops
- 2003-2004: Parttime tutoring of high-school students in Science

Honors and Awards

- KNCV (Dutch Chemical Association) award, first place, 1997 (4000 guilders)
- TURBOMOLE travel grant, 2011-2012 ($ 14500)
- TURBOMOLE GmbH program developer license, 2013-2014
- Travel award from the Gordon Research Conferences' Predominantly Undergraduate Institution Fund ($ 600)
- NSF-RUI award *RUI: SusChEM: Towards accurate computational dynamical and mechanistic studies of transition metal homogeneous (photo)catalysis*, 2015-2018 ($195k)
- Fellow of the Engaged Teaching Fellows Program at MSU, 2015-2016
- Listed as personnel on
  - NSF STEM Pioneers proposal: *A 3-year pilot study to increase science literacy and STEM enrollment among first-year first-generation students*, 2016-2019 ($300k)
  - NSF MRI: *Acquisition of a High Performance Computing Environment for Advancement of Computational Science Research and Education*, 2016-2019 ($497k) PI/Co-PIs: Stefan A. Robila, A. David Trubatch, Chunguang Du.

Current Research Experience

- 2012-: Independent Research at Montclair State University
  - Rational design of catalysts involved in alkane activation
  - Application of the random phase approximation to non-covalent interactions in homogeneous catalysis
  - Development of the random phase approximation (RPA)
    - DFT embedding with RPA
    - *ab initio* molecular dynamics with RPA
  - Excited state mechanisms in isoprene photooxidation in the atmosphere
  - Computational studies of conformationally restricted diamines
- 2009-2012: Postdoctoral research under supervision of Prof. F. U. Furche, University of California, Irvine
  - Development and implementation of methods based on the random phase approximation to describe electron correlation in molecules
  - Application of quantum chemical methods to the study of atmospheric processes, particularly the reaction of NO_2 with water and the formation of brown aerosol, as part of the Atmospheric Integrated Research at the University of California, Irvine institute (AirUCI)
- 2005-2009: PhD research with dr. Fred R. Manby, Bristol University
  - Electronic dynamics of molecules in electric fields using fully propagated time-dependent Hartree-Fock and Kohn-Sham theories

- 2004-2005: Twelve month master project under supervision of dr. Joop H. van Lenthe, Utrecht University
  - The Zeroth-Order Relativistic Approximation (ZORA) method in quantum chemistry: implementation in GAMESS-UK and applications
- 2003-2004: Three months project under supervision of dr. Nico A. J. van Nuland, Utrecht University
  - Elucidating the structure of the SH3 unit using NMR spectroscopy

Publications in Peer-Reviewed Journals

Undergraduate student contributors are highlighted with ⋆

1. *Energies, structures, and harmonic frequencies of small water clusters from the direct random phase approximation.* Julianna Chedid,⋆ Nedjie Jocelyn,⋆ and Henk Eshuis, Journal of Chemical Physics 155, 084303 (2021)
2. *Describing transition metal homogeneous catalysis using the random phase approximation.* Julianna Chedid,⋆ Nashali M. Ferrara,⋆ and Henk Eshuis, Theoretical Chemistry Accounts 137.11, 158 (2018).
3. *Synthesis and computational analysis of conformationally restricted [3.2. 2]-and [3.2. 1]-3-azabicyclic diamines.* Tummalapalli, S. R., Bhat, R., Waitt,⋆ C., Eshuis, H., and Rotella, D. P., Tetrahedron Letters, 58(43), 4087-4089 (2017).
4. *Thermochemistry and Geometries for Transition-Metal Chemistry from the Random Phase Approximation*, Craig Waitt, Nashali M. Ferrara,⋆ and Henk Eshuis. J. Chem. Theory Comp., **12.11**, 5350-5360 (2016)
5. *FDE-vdW: A van der Waals inclusive subsystem density-functional theory*, Kevorkyants, Ruslan and Eshuis, Henk and Pavanello, Michele, J. Chem. Phys., **141**, 044127 (2014)
6. *Analytical first-order molecular properties and forces within the adiabatic connection random phase approximation*, Asbjörn Burow, Jefferson E. Bates, Filipp Furche, and Henk Eshuis, J. Chem. Theory Comp.,**10**,180–194 (2013)
7. *Basis set convergence of molecular correlation energy differences within the random phase approximation*, Henk Eshuis and Filipp Furche, J. Chem. Phys. **136**, 084105 (2012)
8. *Electron correlation methods based on the random phase approximation*, Henk Eshuis, Jefferson E. Bates and Filipp Furche, Theor. Chem. Acc. **131**, 1084 (2012)
9. *A parameter-free density functional that works for noncovalent interactions*, Henk Eshuis and Filipp Furche, J. Phys. Chem. Lett. **2**, 983 (2011)
10. *Fast computation of molecular random phase approximation correlation energies using resolution of the identity and imaginary frequency integration*, Henk Eshuis, Julian Yarkony and Filipp Furche J. Chem. Phys. **132**, 234114 (2010)
11. *The influence of initial conditions on charge transfer dynamics*, Henk Eshuis and Troy van Voorhis, Phys. Chem. Chem. Phys. **11**, 10293 (2009)
12. *Dynamics of molecules in strong oscillating electric fields using time-dependent Hartree-Fock theory*, Henk Eshuis, Gabriel G. Balint-Kurti and Frederick R. Manby, J. Chem. Phys. **128**, 114113 (2008)

13. *The high-resolution NMR structure of the R21A Spc-SH3:P41 complex: Understanding the determinants of binding affinity by comparison with Abl-SH3*, Salvador Casares, Eiso AB, Henk Eshuis, Obdulio Lopez-Mayorga, Nico A. J. van Nuland and Francisco Conejero-Lara, BMC Structural Biology **7**, 22 (2007)

Invited Talks

1. *Capturing weak interactions with the random phase approximation.* TSRC workshop on Excited States and Dynamics, Telluride, Colorado, July 2015

2. *Fast implementation of random-phase approximation for molecular correlation energies: Application to weakly interacting systems, reaction energies and barrier heights.* CE-CAM workshop on Perspectives and Challenges of Many-Particle Methods, University of Bremen, Bremen, Germany, September 2011

3. *Fast implementation of random-phase approximation for molecular correlation energies: Application to weakly interacting systems, reaction energies and barrier heights.* Gordon Research Conference on TDDFT, University of New Hampshire, Biddeford, Maine, USA, August 2011

4. *How accurate is RI-RPA? Quality of resolution-of-the-identity methods for RPA correlation energies.* Multidisciplinary Workshop on RPA, Paris, France, January 2010

5. *Electronic dynamics of molecules in strong electric fields, and charge transfer dynamics using time-dependent Hartree-Fock theory.* Centre for Computational Chemistry super group meeting, Bristol University, UK, December 2008

6. *Electronic dynamics of molecules in strong electric fields, and charge transfer dynamics using time-dependent Hartree-Fock theory.* Seminar, UCI Chemistry, Irvine, USA, September 2008

Contributed Talks and Posters

1. *Applications of the random phase approximation to transition metal chemistry*, Henk Eshuis, Virtual Group meeting presentation for the Furche group at the University of California, Irvine, USA, June 2020

2. *The random phase approximation: a functional that works for transition metal chemistry*, Craig Waitt, Kelsey Orzel, Julianna Chedid and Henk Eshuis, ACS national meeting, Orlando, Florida, USA, April 2019

3. *Describing water clusters using the random phase approximation*, Julianna Chedid, Kelsey Orzel and Henk Eshuis, ACS national meeting, Orlando, Florida, USA, April 2019

4. *The random phase approximation, a functional that works for transition metal chemistry*, Henk Eshuis, Bristol University, CCC group talk, Bristol, UK, March 2018

5. *Performance of the Random Phase Approximation for first-row transition metal catalysis*, Henk Eshuis, WATOC, Munich, Germany, August 2017

6. *RIRPA-based Ab Initio Molecular Dynamics; Acetylene Trimerization of CpCo Catalytic System*, Ryan Dykstra* and Henk Eshuis, Student Research Symposium, Montclair State University, April 2016

7. *Photoactivation of CF_3I in the presence of photoexcited $Ru(bpy)_3^+$* Julianna Chedid* and Henk Eshuis, Student Research Symposium, Montclair State University, April 2016

8. *The random phase approximation for transition metal chemistry* Anthony Strobolakos,* Olivia Perez,* Nashali Ferrara,* Craig Waitt* and Henk Eshuis, Rutgers University Newark, Computational Chemistry seminar, Newark, October 2015

9. *Accurate Determination of Interaction Energies Using the Random Phase Approximation for Problematic Dispersion-Bond Complexes*, Craig Waitt* and Henk Eshuis, Student Research Symposium, Montclair State University, April 2015

10. *Random Phase Approximation for Problematic Dispersion-Bound Complexes* Craig Waitt* and Henk Eshuis, Novel Tools in Computational Chemistry Coding workshop, Rutgers University Newark, Newark, April 2015

11. *Developing the random phase approximation into a practical electronic structure method*, Henk Eshuis, Rutgers University Newark, Newark, November 2014

12. *The random phase approximation and transition metal chemistry*, Olivia Perez,* Anthony Strobolakos* and Henk Eshuis, Gordon Research Conference on Computational Chemistry, West Dover, VT, July 2014

13. *Improved computational results for transition metal chemistry*, Nashali Ferrara* and Henk Eshuis, Student Research Symposium, Montclair State University, April 2014

14. *The random phase approximation: a parameter-free functional that works for non-covalent interactions*, Henk Eshuis, Asbjörn Burow, Jefferson E. Bates and Filipp Furche, Bristol-Myers Squibb, NJ, February 2014

15. *Towards use of the random phase approximation for transition metal chemistry*, Olivia Perez,* Anthony Strobolakos* and Henk Eshuis, Gordon Research Conference on TDDFT, Biddeford, ME, August 2013

16. *Capturing weak interactions in chemistry*, Andrew Hernandez,* Anthony Strobolakos,* Andrew Vild* and Henk Eshuis, 2013 Student Research Symposium, Montclair State University, April 2013

17. *Developing the random phase approximation into a useful quantum chemistry method*, Henk Eshuis, Asbjörn Burow, Jefferson E. Bates, and Filipp Furche, Center for Functional Nanomaterials, Brookhaven National Lab, January 2013

18. *Developing the random phase approximation into a useful quantum chemistry method*, Henk Eshuis, Asbjörn Burow, Jefferson E. Bates, and Filipp Furche, Theoretial and applied quantum matter physics Seminar, Graduate Center, CUNY, New York City, October 2012

19. *The random phase approximation for electron correlation: fast implementation, and application*, Henk Eshuis and Filipp Furche, 52nd Sanibel Symposium, St. Simons Island, Georgia, February 2012

20. *Implementation of analytical gradients for the random phase approximation*, Henk Eshuis and Filipp Furche, ACS meeting, San Diego, March 2012

21. *Molecular correlation energies from the random phase approximation: fast implementation, applications and basis set convergence*, Henk Eshuis and Filipp Furche, LUEST workshop, Telluride, June 2012

22. *RIRPA: fast implementation and applications*, Henk Eshuis and Filipp Furche, Gordon Research Conference on TDDFT, University of New England, Biddeford, Maine, 2011

23. *Fast implementation of random-phase approximation for molecular correlation energies: Application to weakly interacting systems.* ACS national meeting, Anaheim, USA, March 2011

24. *Computational Clues on the Brown Color of Secondary Organic Aerosols.* 7th annual international AirUCI workshop, Laguna Beach, USA, January 2011

25. *Atmospheric HONO Generation from Excited NO_2 and Water: A Computational Study.* 7th annual international AirUCI workshop, Laguna Beach, USA, January 2011

26. *Implementation and performance of the random-phase approximation for molecular electron correlation energies.* TURBOMOLE workshop, Erkner, Germany, October 2010

27. *Testing the RI-RPA method: quality of the integration scheme and of reaction energies*, Henk Eshuis and Filipp Furche, CECAM workshop on 'van der Waals forces in DFT, RPA and beyond', Lausanne, Switzerland, June 2010

28. *Formation of HONO from electronically excited NO_2 and H_2O*, Zenghui Yang, Henk Eshuis, Barbara Finlayson-Pitts and Filipp Furche, AirUCI poster session, University of California, Irvine, May 2010

29. *Reactions of Excited NO_2 as a HONO Source in Ambient Air.* 6th annual international AirUCI workshop, Laguna Beach, USA, January 2010

30. *Electronic dynamics of molecules in strong electric fields*, Henk Eshuis, Frederick R. Manby, Gordon Research Conference on TDDFT, Colby-Sawyer College, New Hampshire, July 2009

31. *Electronic dynamics of molecules in strong electric fields*, Henk Eshuis, Gabriel G. Balint-Kurti, Frederick R. Manby, CMS, Cirencester, June 2008

32. *Electronic dynamics using time-dependent Hartree-Fock theory: Molecules in strong electric fields, and charte transfer*, CoCoChem meeting, University of Birmingham, UK, April 2008

33. *Electronic dynamics of molecules in strong electric fields, and charge transfer dynamics using time-dependent Hartree-Fock theory.* Van Voorhis group meeting, M.I.T., USA, March 2008

34. *Time-dependent Hartree-Fock theory for real time dynamics of molecules in strong electric fields*, South-West Computational Chemistry meeting, Cardiff University, September 2007

35. *Molecules in strong electric fields: Time-dependent Hartree-Fock simulations*, Henk Eshuis, Gabriel G. Balint-Kurti, Frederick R. Manby, Gordon Research Conference on TDDFT, Colby College, Maine, July 2007

Affiliations

- Member of the American Chemical Society, Computers in Chemistry Division