

VU Research Portal

Molecular properties in the linear response regime and beyond with relativistic coupled-cluster

Yuan, Xiang

2024

DOI (link to publisher)

[10.5463/thesis.505](https://doi.org/10.5463/thesis.505)

document version

Publisher's PDF, also known as Version of record

[Link to publication in VU Research Portal](#)

citation for published version (APA)

Yuan, X. (2024). *Molecular properties in the linear response regime and beyond with relativistic coupled-cluster*. [PhD-Thesis - Research and graduation internal, Vrije Universiteit Amsterdam]. <https://doi.org/10.5463/thesis.505>

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

Take down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

E-mail address:

vuresearchportal.ub@vu.nl

Outline

Abstract	xv
Acknowledgements	xvii
Outline	xix
List of publications	xxi
Introduction	1
I Methodology	7
1 Electronic Structure Theory	9
2 Response Theory	27
II ExaCorr Implementation	39
3 Implementation of Linear Response properties based on Relativistic Coupled Cluster Theory	41
4 Implementation of Quadratic Response Properties based on Relativistic Equation-of-Motion Coupled Cluster Theory	103
5 Note: Reimplementation of Ionization Potential, and Electron Affinity based upon Relativistic Equation-of-Motion Coupled Cluster	143
6 Reduced-Scaling: Relativistic MP2 Frozen Natural Orbitals	153
III Applications on molecules containing heavy elements	171

7 Papers of application works	173
Summary and Conclusion	203
Bibliography	207
A Supplemental information of Chapter 3	219
B Supplemental information of Chapter 4	241
C Supplemental information of Chapter 6	247
D Supplemental information of Chapter 7	253