Curriculum Vitae

Gianluca Levi, January 18, 2024

Home Address	Grundarstígur 9, 101 Reykjavík, Iceland
Office Address	Háskóli Íslands (University of Iceland), VR-III Hjarðarhagi 2, 107 Reykjavík
Born	June 17, 1990
Nationality	Italian
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RESEARCH PROFILE AND GRANTS

Computational and theoretical physical chemistry with a focus on excited electronic states and photoinduced chemical dynamics. Development of density functional theory approaches for excited states and multiscale molecular dynamics methods. Time-resolved spectroscopy and scattering experiments at large scale synchrotron and free electron laser facilities with experimental collaborators. Main areas of applications are photocatalysis and solar energy conversion.

ORCID:	0000-0002-4542-0653
Web of Science ResearcherID:	GYQ-9226-2022
Scopus Identifier:	57199649322

Research grants from competitive funds

2021 - 2024 **Project grant, Icelandic Research Fund**

Project title	*Ultrafast Charge and Energy Transfer in Sunlight Conversion* (CNERGY)
Role	Principal investigator
Grant amount	360.190 Euros (including overhead)

2019 - 2021 **Postdoctoral Fellowship Grant, Icelandic Research Fund**

Project title	*Electron-Nuclear Dynamics in Iron-Sensitized Solar Cells: A Unified Model Description from Light Absorption to Charge Separation*
Role	Principal investigator
Grant amount	224.240 Euros (including overhead)

2021 **Student Innovation Fund, Icelandic Centre for Research**

Project title	*Efficient Organic Solar Cells*
Role	Supervisor
Grant amount	4.080 Euros

EMPLOYMENT AND EDUCATION

Current and previous positions

2021 - **Group leader**
Science Institute of the University of Iceland (Raunvísindastofnun Háskólans)

2018 - 2021 **Postdoctoral researcher**
Science Institute of the University of Iceland (Raunvísindastofnun Háskólans)

Education

2014 - 2018 **PhD**
Department of Chemistry, Technical University of Denmark (DTU)

Funding	Academic Excellence Scholarship
Thesis title	*Photoinduced Molecular Dynamics in Solution: Multiscale Modelling and the Link to Ultrafast Experiments*
Supervisors	Prof. Klaus B. Møller, Prof. Niels E. Henriksen, Dr. Asmus O. Dohn

2012 - 2014 **Master of Science in Chemistry**
Polytechnic and Basic Sciences School, University of Naples Federico II

Final grade	110/110 & lode
Thesis title	*Oxidation of solid carbon materials: structural and thermochemical analysis*
Supervisors	Prof. Mauro Causà, Prof. Piero Salatino and Dr. Osvalda Senneca

2009 - 2012 **Bachelor of Science in Chemistry**
Department of Chemistry, University of Naples Federico II

Final grade	110/110 & lode
Thesis title	*Thermodynamic Study of the Metal-Water-Nicotine System*
Supervisor	Prof. Carla Manfredi

Other Qualifications

Nov 2020 **American Chemical Society Reviewer Lab**
Online course on peer review of scientific publications

TEACHING AND SUPERVISION

Teaching activities

2022 - **Lecturer**

Institution	University of Iceland, Department of Chemistry
Role	Independent design of lectures and exercises
Level	Graduate and undergraduate students in chemistry, biochemistry and chemical engineering

Molecular Spectroscopy and Reaction Dynamics (8/10 ECTS)
Physical Chemistry A (6 ECTS)
Computational Chemistry (8/10 ECTS)

2023 **External teacher**

Institution	Technical University of Denmark, Department of Physics
Role	Hands-on teaching and design of computer exercises
Level	Master degree in Physics

Special course on *Molecular Dynamics and X-ray Scattering Simulations* (5 ECTS)

2015 - 2016 **Teaching assistant**

Institution	Technical University of Denmark, Department of Chemistry
Role	Assisting students with problem solving and design of computer exercises
Level	Graduate and undergraduate students in chemistry and chemical engineering

Physical Chemistry 3 (5 ECTS)
Applied Computational Chemistry (5 ECTS)

Supervision of students and postdoctoral fellows

2021 - **One Postdoc**
Supervision of Dr. Elli Selenius within the project CNERGY funded by the Icelandic Research Fund (University of Iceland)

2020 - **Two PhD students**
Co-supervision of Yorick L. A. Schmerwitz and Benedikt O. Birgisson (University of Iceland)

2023 **Two Master students**
Co-supervision of Magnus A. H. Christiansen (Technical University of Denmark) and Alec E. Sigurðarson (University of Iceland)

RESEARCH ACTIVITIES

Beamtimes awarded for experiments at large scale facilities

Nov 2022 **XFEL ultrafast X-ray solution scattering at XFEL**

Experiment title	*Photoinduced intramolecular and solvation dynamics of an organic chromophore in polar solvent*
Facility	SwissFEL X-ray free-electron laser at the Paul Scherrer Institute
Role	Principal investigator, coordination and data analysis

Oct 2022 **XFEL ultrafast X-ray solution scattering at XFEL**

Experiment title	*Photoinduced intramolecular and solvation dynamics of an organic chromophore in polar solvent*
Facility	European X-ray free electron laser
Role	Main proposer, coordination and data analysis

Sep 2022 **Synchrotron time-resolved X-ray solution scattering**

Experiment title	*Imaging photoinduced isomerization and solvation dynamics during intramolecular charge transfer in an organic chromophore via time-resolved X-ray scattering*
Facility	Advanced Photon Source synchrotron, Argonne National Laboratory

Role	Principal investigator, coordination and data analysis

Research Stays

Study visits

Mar 2017 Faculty of Physical Sciences, University of Iceland
Visits as PhD student to the group of Prof. Hannes Jónsson

Short research visits

Jan 2023 Laboratoire de Chimie et Physique Quantiques (LCPQ), Université Paul Sabatier (Toulouse)
Visit to the groups of Dr. Pierre-Francois Loos and Dr. Isabelle Dixon, taking part in scientific discussions and giving a seminar

Oct 2022 Department of Physics, Technical University of Denmark
Visit to the groups of Prof. Martin M. Nielsen and Dr. Kristofffer Haldrup within a collaboration on X-ray scattering studies of solvated molecules

Aug 2018 Department of Materials Science, University of Milano-Bicocca (Italy)
Giving a seminar and taking part in scientific discussions in the group of Prof. Cristiana Di Valentin

Publications

I have authored one monograph and 21 scientific articles (19 already published in peer-reviewed journals indexed in the Web of Science Core Collection and two currently under review and available as preprints on arXiv). The publications include three last author articles, seven corresponding author publications, and two Editor's suggestion (*J. Chem. Phys.* 2023 and *Phys. Rev. Lett.* 2019). Number of citations: 524 (Google Scholar), 392 (Web of Science), 412 (Scopus). H-index: 12 (Google Scholar), 10 (Web of Science), 10 (Scopus). See the complete list of publications at the end of the CV.

Reviewing activity

Peer review of two scietific articles for ACS journals *J. Phys. Chem. Lett.* and *J. Org. Chem.*.

Talks at Conferences and Seminars

Eight academic seminars, three invited and seven selected talks at international scientific conferences.

Nov 2023 Icelandic research e-infrastructure (IREI) conference, University of Iceland
Invited talk

Aug 2023 15th Femtochemistry Conference, Freie Universität Berlin
Selected talk

Apr 2023 Workshop on Emerging Excited State Methods in Electronic Structure, Pierre-Francois Loos's group at Université Paul Sabatier (Toulouse)
Invited talk

Jan 2023 Laboratoire de Chimie et Physique Quantiques (LCPQ) seminar, Université Paul Sabatier (Toulouse)

Seminar

Jul 2022 Symposium on New Strategies for Solving the Kohn-Sham Equations, Conference on Scientific Computation and Differential Equations (SciCADE), University of Iceland
Selected talk

Mar 2022 Developments in Hybrid QM/QM, QM/MM, and Fragmentation Methods symposium, American Chemical Society March meeting, San Diego
Selected talk

Mar 2022 Density functional theory and beyond symposium, American Physical Society March meeting, Chicago
Selected talk

Nov 2021 Chemistry-Biochemistry Seminar Series, University of Iceland
Online seminar

Nov 2021 Quantum Molecular Dynamics (QMD) seminar, University of Edinburgh
Online seminar

Jun 2021 GPAW 2021: Users and Developers Meeting, online
Invited talk

May 2021 Quantum Dynamics and Spectroscopy of Functional Molecular Materials and Biological Photosystems, Les Houches workshop 2021, online
Selected talk

Nov 2020 Computational Atomic-scale Materials Design (CAMD) seminar, DTU Physics
Online seminar

Sep 2020 New horizons in density functional theory Faraday Discussion conference, online
Selected talk

Nov 2019 Young Academics of Háskóli Ísland (YAHI) seminar series, University of Iceland
Seminar

Nov 2018 Chemistry-Biochemistry Seminar Series, University of Iceland
Seminar

Aug 2018 Prof. Cristiana Di Valentin's group at the Department of Materials Science, University of Milano-Bicocca
Seminar

Jul 2017 22nd International Symposium on Photochemistry and Photophysics of Coordination Compounds (ISPPCC 2017), Oxford
Selected talk

Mar 2017 Prof. Hannes's Jónsson's group at University of Iceland
Seminar

OTHER CONTRIBUTIONS TO THE RESEARCH COMMUNITY

Organization of scientific meetings

Jul 2022 Main organizer of symposium on *New Strategies for Solving the Kohn-Sham Equations* Conference on Scientific Computation and Differential Equations (SciCADE) at the University of Iceland

Code development in open-source software

I am one of the main developers of the GPAW open-source program for electronic structure calculations and an active contributor of the Atomic Simulation Environment (ASE) for atomic calculations. All developed code is freely available on gitlab, either on personal (https://gitlab.com/theochem-ui) or official (https://gitlab.com/gpaw/gpaw, https://gitlab.com/ase/ase) repositories.

AWARDS

- Springer Thesis Award 2019. Monetary award and publication of the PhD thesis in the series *Springer Theses: Recognizing Outstanding Ph.D. Research* (10.1007/978-3-030-28611-8).
- Prize *Premio Università Paolo Iannotti 2015 Laureati Eccellenti* awarded by the Ateneapoli magazine to students in Universities in Campania (Italy) who excel in their academic studies.

COMPLETE PUBLICATION LIST

Monographs

[1] G. Levi. *Photoinduced Molecular Dynamics in Solution*. Springer Theses - Recognizing Outstanding Ph.D. Research. Springer, Cham, 2019.

Publications

[1] E. Selenius, A. Elías Sigurðarson, Y. L. A. Schmerwitz, and **G. Levi**. Orbital optimized vs time-dependent density functional calculations of intramolecular charge transfer excited states. *Journal and Chemical Theory and Computation (submitted), arXiv.2311.01604*, 2023.

[2] J. J. Mortensen, A. H. Larsen, M. Kuisma, A. V. Ivanov, A. Taghizadeh, A. Peterson, A. Haldar, A. O. Dohn, C. Schaefer, E. Ö. Jónsson, E. Hermes, F. A. Nilsson, G. Kastlunger, **G. Levi**, H. Jónsson, H. Häkkinen, J. Fojt, J. Kangsabanik, J. Sødequist, J. Lehtomäki, J. Heske, J. Enkovaara, K. T. Winther, M. Dulak, M. Melander, M. Ovesen, M. Louhivouri, M. Walter, M. Gjerding, O. Lopez-Acevedo, P. Erhart, R. Warmbier, R. Würdermann, S. Kaappa, S. Latini, T. M. Boland, T. Bligaard, T. Skovhus, T. Susi, T. Maxson, T. Rossi, X. Chen, Y. L. A. Schmerwitz, J. Schiøtz, T. Olsen, K. W. Jacobsen, and K. S. Thygesen. Gpaw: open python package for electronic-structure calculations. *J. Chem. Phys. (submitted), arXiv:2310.14776*, 2023.

[3] A. E. Sigurðarson, Y. L. A. Schmerwitz, D. K. V. Tveiten, **G. Levi**, and H. Jónsson. Orbital-optimized Density Functional Calculations of Molecular Rydberg Excited States with Real Space Grid Representation and Self-Interaction Correction. *Journal of Chemical Physics*, 159:214109, 2023. *Editors' Suggestion*.

[4] T. Katayama, T. K. Choi, D. Khakhulin, A. O Dohn, C. J. Milne, G. Vankó, Z. Németh, F. A. Lima, J. Szlachetko, T. Sato, S. Nozawa, S. I. Adachi, M. Yabashi, T. J. Penfold, W. Gawelda, and **G. Levi**.

Atomic-scale observation of solvent reorganization influencing photoinduced structural dynamics in a copper complex photosensitizer. *Chemical Science*, 14:2572–2584, 2023.

[5] A. V Ivanov, Y. L. A. Schmerwitz, **G. Levi**, and H. Jónsson. Electronic excitations of the charged nitrogen-vacancy center in diamond obtained using time-independent variational density functional calculations. *SciPost Phys.*, 15:009, 2023.

[6] Y. L. A. Schmerwitz, **G. Levi**, and H. Jónsson. Calculations of Excited Electronic States by Converging on Saddle Points Using Generalized Mode Following. *Journal of Chemical Theory and Computation*, 19(12):3634–3651, 2023.

[7] Y. L. A. Schmerwitz, A. V. Ivanov, E.Ö. Jónsson, H. Jónsson, and **G. Levi**. Variational Density Functional Calculations of Excited States: Conical Intersection and Avoided Crossing in Ethylene Bond Twisting. *Journal of Physical Chemistry Letters*, 13:3990–3999, 2022.

[8] A. V. Ivanov, **G. Levi**, E. Ö. Jónsson, and H. Jónsson. Method for Calculating Excited Electronic States Using Density Functionals and Direct Orbital Optimization with Real Space Grid or Plane-Wave Basis Set. *Journal of Chemical Theory and Computation*, 17(8):5034–5049, 2021.

[9] **G. Levi**, A. V. Ivanov, and H. Jónsson. Variational Density Functional Calculations of Excited States via Direct Optimization. *Journal of Chemical Theory and Computation*, 16(11):6968–6982, 2020.

[10] **G. Levi**, A. V. Ivanov, and H. Jonsson. Variational Calculations of Excited States Via Direct Optimization of Orbitals in DFT. *Faraday Discussions*, 224:448, 2020.

[11] J. G. Brandenburg, K. Burke, E. Fromager, M. Gatti, S. Giarrusso, N. I. Gidopoulos, P. Gori-Giorgi, D. Gowland, T. Helgaker, M. J. P. Hodgson, L. Lacombe, **G. Levi**, P.-F. Loos, N. T. Maitra, E. Maurina Morais, N. Mehta, F. Monti, M. R. Mulay, K. Pernal, L. Reining, P. Romaniello, M. R. Ryder, A. Savin, D. Sirbu, A. M. Teale, A. J. W. Thom, D. G. Truhlar, J. Wetherell, and W. Yang. New approaches to study excited states in density functional theory: general discussion. *Faraday Discussions*, 224:483–508, 2020.

[12] **G. Levi**, M. Causà, L. Cortese, P. Salatino, and O. Senneca. On how mild oxidation affects the structure of carbons: Comparative analysis by different techniques. *Applications in Energy and Combustion Science*, 1-4:100006, 2020.

[13] **G. Levi**, E. Biasin, A. O. Dohn, and H. Jónsson. On the interplay of solvent and conformational effects in simulated excited-state dynamics of a copper phenanthroline photosensitizer. *Physical Chemistry Chemical Physics*, 22:748–757, 2020.

[14] K. Haldrup, **G. Levi**, E. Biasin, P. Vester, M. G. Laursen, F. Beyer, K. S. Kjær, T. B. Van Driel, T. Harlang, A. O. Dohn, R. J. Hartsock, S. Nelson, J. M. Glownia, H. T. Lemke, K. J. Gaffney, N. E. Henriksen, K. B. Møller, and M. M. Nielsen. Ultrafast x-ray scattering measurements of coherent structural dynamics on the ground-state potential energy surface of a diplatinum molecule. *Physical Review Letters*, 122:063001, 2019. *Editors' Suggestion*.

[15] M. Abedi, **G. Levi**, D. B. Zederkof, N. E. Henriksen, M. Pápai, and K. B. Møller. Excited-state solvation structure of transition metal complexes from molecular dynamics simulations and assessment of partial atomic charge methods. *Phys. Chem. Chem. Phys.*, 21:4082–4095, 2019.

[16] M. Pápai, M. Abedi, **G. Levi**, E. Biasin, M. M. Nielsen, and K. B. Møller. Theoretical Evidence of Solvent-Mediated Excited-State Dynamics in a Functionalized Iron. *The Journal of Physical Chemistry C*, 2019.

[17] **G. Levi**, M. Pápai, N. E. Henriksen, A. O. Dohn, and K. B. Møller. Solution structure and ultrafast vibrational relaxation of the PtPOP complex revealed by ΔSCF-QM/MM Direct Dynamics simulations. *Journal of Physical Chemistry C*, 122:7100–7119, 2018.

[18] E. Biasin, T. B. van Driel, **G. Levi**, M. G. Laursen, A. O. Dohn, A. Moltke, P. Vester, F. B. K. Hansen, K. S. Kjaer, R. Hartsock, M. Christensen, K. J. Gaffney, N. E. Henriksen, K. B. Møller, K. Haldrup, and M. M. Nielsen. Anisotropy enhanced X-ray scattering from solvated transition metal complexes. *Journal of Synchrotron Radiation*, 25(2):306–315, 2018.

[19] A. O. Dohn, E. Ö. Jónsson, **G. Levi**, J. J. Mortensen, O. Lopez-Acevedo, K. S. Thygesen, K. W. Jacobsen, J. Ulstrup, N. E. Henriksen, K. B. Møller, and H. Jónsson. Grid-Based Projector Augmented Wave (GPAW) implementation of Quantum Mechanics/Molecular Mechanics (QM/MM) electrostatic embedding and application to a solvated diplatinum complex. *Journal of Chemical Theory and Computation*, 13(12):6010–6022, 2017.

[20] **G. Levi**, M. Causà, P. Lacovig, P. Salatino, and O. Senneca. Mechanism and Thermochemistry of Coal Char Oxidation and Desorption of Surface Oxides. *Energy & Fuels*, 31:2308–2316, 2017.

[21] **G. Levi**, O. Senneca, M. Causà, P. Salatino, P. Lacovig, and S. Lizzit. Probing the chemical nature of surface oxides during coal char oxidation by high-resolution XPS. *Carbon*, 90:181–196, 2015.