CURRICULUM VITAE Kathrin Helen Hopmann

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RESEARCH & EXPERTISE

I have 20 years of research experience from different areas of chemistry, including molecular biology, biochemistry, computational chemistry, spectroscopy and organometallic chemistry. My main research goal is to understand how molecules work and how they can be tuned towards specific applications. Since 2014, I lead my own research group, which is investigating and designing metal catalysts. I am leader of an H2020-Innovative Training Network and a NordForsk University Hub, and Associate Editor of the journal *Organometallics.* I have extensive experience with external research funding and have attracted >5 M€ funding for personal projects, and >29 M€ in collaboration with others from local, national, Scandinavian and European research agencies. I am a dedicated team worker, a supportive supervisor, a diligent administrator, and a skilled writer & communicator.

CURRENT AND PREVIOUS SCIENTIFIC POSITIONS

2018 –	**Associate Editor for *Organometallics***, ACS, USA, part-time
2018 –	**Assoc. Professor**, Dept. of Chemistry, UiT The Arctic University of Norway, full-time
2011 – 2018	**Researcher,** Dept. of Chemistry, UiT, Norway. Permanent during 2014-18, full-time
2009 – 2011	**User & software support**, High Performance Computing group, UiT, Norway, part-time
2008 – 2011	**Postdoc,** Center for Theoretical & Computational Chemistry, UiT, Norway, full-time
2004 – 2008	**Doctoral Fellow**, Dept. of Theoretical Chem., Royal Institute of Technology, SE, full-time
2004	**Scientific Fellow Structural Biology**, Karolinska Institute. SE, full-time

EDUCATION

2015	**Leadership program** for young research talents, UiO, Norway
2015	**Basic pedagogic competence** (digitalmappe.uit.no/kathrinhopmann), UiT, Norway
2008	**Ph.D.** in Biotechnology, Dept. of Theoretical Chemistry, KTH-Royal Institute of Technology, Sweden (Supervisor: Prof. F. Himo). Disputation Date: *04.04.2008*
2007	**Licentiate** in Biotechnology, Dept. of Theoretical Chemistry, KTH, Sweden
2002	**B.Sc.** in Chemistry/Molecular Biology, Aarhus University, Denmark (grade 13 of 13)

RECENT STUDENT SUPERVISION & OTHER GROUP MEMBERS (from 2015, UiT)

2020 –	Main supervisor of PhD student **Jhonnatan Carvalho** (computational)
2020	Co-supervisor of admin **Trine Andreassen** (administrative staff)
2020 –	Co-supervisor of admin **Marie-Josée Haglund Halsør** (administrative staff)
2020	Main supervisor of BSc. student **Kristine Rein** (computational). Thesis delivered 01.06.20
2019 –	Main supervisor of PhD student **Dat Do Cuong** (computational)
2019	Co-supervisor of researcher **Sietske Grijseels** (experimental)
2018 – 2020	Main supervisor of postdoc **Diego Garcia-Lopez** (computational)
2018 –	Co-supervisor of postdoc **Ashot Gevorgyan** (experimental)
2018	Co-supervisor of Bachelor student **Louise Poutot** (computational, Uni. Franche-Comte France)
2017 –	Main supervisor of PhD student **Anders M. Brakestad** (computational)
2017 – 2020	Main supervisor of engineer/adm **Yngve Guttormsen** (experimental & administrative)
2017 – 2020	Main supervisor of PhD student **Marc Obst** (computational). PhD Defense: 04.09.2020
2016 – 2020	Main supervisor of PhD student **Ljiljana Pavlovic** (computational). PhD Defense: 21.08.2020
2016 – 2019	Co-supervisor of postdoc **Janakiram Vaitla** (experiment. Now faculty member at IIT Delhi)
2016 – 2017	Co-supervisor of MSc. student **Kristers Ozols** (computational, Riga Technical Uni., Latvia)
2015 – 2018	Main supervisor of postdoc **Glenn Morello** (computational. Now faculty member at VSCU)
2015	Main supervisor of computational project (exchange student **Sonja Tischlik**, Master level)

AWARDED GRANTS

Year	Title	Funds	Funding Source	Grant Type (webpage)	My role
2020-24	***CATCHME:*** *CATCH ME IF YOU CAN: Selective CO_2 conversion via chiral CO_2 trapping*	1.2 M€	• Research Council of Norway	Personal FriPro Researcher Grant to me	• **Project Leader** • Wrote application
2020-24	***CO_2PERATE****: Cooperation towards a sustainable chemical industry*	4.2 M€	• European Commission	Innovative Training Network (co2perate.eu)	• **Coordinator** • 1 of 10 PIs • Wrote application
2019-21	***OILFREE:*** *Oilfree Chemistry*	0.4 M€	• UiT	Research & Network	• 1 of 3 PIs • Wrote application
2019-21	***CESSY:*** *Catalytic enantioselective sigmatropic rearrangements of vinyl sulfonium ylides*	0.35 M€	• Research Council of Norway	FriPro mobility grant for a researcher in my group	• Co-supervisor • Co-wrote application
2018-23	***NordCO₂****: Nordic Consortium for CO_2 Conversion*	6.6 M€	• NordForsk (2.1M€) and 9 Universities (4.5 M€)	Research & Network, (site.uit.no/nordco₂)	• **Coordinator** • 1 of 12 PIs • Wrote application
2018-21	***iCCU****: Transforming CO_2 to capi-tal by interdisciplinary CCU*	2 M€	• UiT	Research & Network (site.uit.no/iCCU)	• 1 of 5 PIs • Co-wrote application
2017-27	***Hylleraas*** *Centre for Quantum Molecular Sciences*	14 M€	• Research Council of Norway	Centre of Excellence (hylleraas.no)	• 1 of 6 PIs* • Co-wrote application
2017-21	***CHOCO****: Sustainable catalysts for homogeneous CO_2 conversion*	2.9 M€	• Tromsø Research Foundation (1.5 M€) & UiT (1.4 M€)	Personal Recruitment Grant to me (site.uit.no/choco)	• **Project Leader** • Wrote application
2015-23	***BioCat****: National PhD school in biocatalysis*	2.4 M€	• Research Council of Norway	PhD School (site.uit.no/biocat)	• Teaching • Co-wrote application
2015-19	***Marval****: From unexploited marine biomass to high value products*	2 M€	• UiT	Research & Network (site.uit.no/marval)	• 1 of 6 PIs • Co-wrote application
2014-20	*CPU hours, annual quota*	2 MCPU	• Sigma2	Personal CPU Grant	• Wrote application
2014-18	***deFacto****:Selectivity-determining factors in asymmetric catalysis*	0.6 M€	• Research Council of Norway	Young Research Talent Grant	• **Project Leader** • Wrote application

* PI during 2017 – 2020.

AWARDS OTHER THAN GRANTS

2018 - 2020 Membership in the UiT *AURORA Program for outstanding scientists*
2018 *UiT - Equality Prize 2018*, 5000 €.
2017 *UiT - Young Researcher Prize 2017*, 5000 €.

COMMISSIONS OF TRUST

2020 – Member of International Advisory Board of WIRES – Computational Molecular Science
2020 – Coordinator of ITN network CO_2PERATE
2019 External examiner of applications in C1 Value Academy Programme, Academy of Finland
2019 External examiner of PhD thesis (D. Ascough), Oxford University, England
2019 Member of the National resource allocation committee for e-infrastructure, Norway
2018 – Associate Editor of ACS journal *Organometallics* (USA). Journal impact factor ca 4.
2018 – 2020 Leader of the University Hub Nordic Consortium for CO_2 Conversion
2018 – 2019 Member of the leadership team of the Arctic Centre for Sustainable Energy, UiT
2018 – Initiator & interim leader of the UiT Academy for Women in Research and Arts, UiT
2017 Co-organizer of the March For Science Norway and leader of the Tromsø section
2017 Committee member for evaluation of a PhD dissertation at Uppsala University, SE
2016 – 2017 Board member Norwegian Graduate school in Biocatalysis (BioCat)
2015 Guest editor of Special Issue of *Int. J. Quantum Chem*.
2014 Examiner PhD thesis, Dept. Phys. Chem., University of the Free State, South Africa
2013 – 2019 Board member (2013-17) and Deputy board member (2018-19), Dept. of Chemistry, UiT
2013 – 2017 Study Board Member, Dept. of Chemistry, UiT
2012 – Peer-reviewer for *Angewandte Chemie, Chem. Comm., Nature Chem., Nature Comm., J. Phys. Chem., J. Org. Chem., ACS Catalysis, JCTC, JACS, Science, Dalton Trans., Organomet., Chem. Eur. J., ChemCatChem., PCCP, Research & Change.*

INSTITUTIONAL RESPONSIBILITIES (all at UiT)

2010 – 2020 Leader of 16 and member of 5 committees for evaluation of PhD/Post doc/admin applications
2018 Member of the research strategy committee at Dept. of Chemistry, UiT
2015 – 2017 Committee member for restructuring department facilities, Dept. of Chemistry, UiT
2015 Committee member for social activities & for internal evaluation of funding applications
2014 – 2017 Initiator & leader of bimonthly meetings of departmental researchers on career development
2011 – 2013 Leader of 2 committees for evaluation of PhD dissertations

TEACHING AND OUTREACH ACTIVITIES (all at UiT)

2020 Development & teaching of PhD course ***Responsible Research and Innovation*** (part of CO_2perate ITN).
2019 Seminar teacher & preparation of material, BSc. course *Organic chemistry*, KJE-1002
2018 – 2020 Lecturer & seminar teacher, MSc. course *From quantum mechanics to medicine*, KJE-3001
2018 Development + teaching of PhD course *Mechanisms for CO_2 activation*
2018 Organizer of PhD course *Python programming for beginners*
2018 Development & organization of large outreach event *CO_2 Days*
2018 Development & organization of exhibition *Did you think?* on females in STEM subjects
2016 – 2017 Development & teaching *Enzyme mechanisms*, KJE-8705, BioCat PhD school
2016 Seminar teacher for PhD course ***Scientific writing***, FSK-8002, High North Academy
2014 – Internet-based outreach via Facebook (@CHOCO.UiT, @UiTawora, @CO_2perateITN), Twitter (@NordCO_2, @CO_2perate_ITN) & Web pages (site.uit.no/choco, site.uit.no/nordco$_2$, co$_2$perate.eu)
2014,15,19 Co-organizer of local chemistry stand at annual Norwegian national science festival
2014 Lecturer & seminar teacher for BSc. course *General chemistry*, KJE-1001
2013 – 2018 Responsible for development + teaching of ***Inorganic chemistry for teachers***, KJE-6004
2013 – 2017 Lecturer & seminar teacher in *Science education for teachers*, MNF-6001
2009 – 2019 Lecturer & seminar teacher in MSc./PhD course *Computational chemistry*, KJE-3102

RECENT INVITED TALKS (selected, for more comprehensive list see site.uit.no/choco/conferences)

2021 *Upcoming*: Invited speaker, Hengstberger Symposium on "*Element-Ligand Cooperativity: Unifying the concepts from d-block and p-block chemistry*", Heidelberg, Germany, 8-10.9.
2020 Invited speaker, Webinar series, Department of Chemistry, IIT Dehli, 10.12.
2019 Invited speaker *Inter. Society for Theoretical Chemical Physics*, Tromsø, Norway, 11-17.7.
2019 Plenary speaker *European Conference on Organomet. Chem.*, Helsinki, Finland, 16-20.6.
2018 Invited speaker *National Meeting of the Norwegian Chem. Society*, Norway, 16-18.10.
2018 Invited speaker *ACS Forum: Celebrating Diversity in Inorg./Org. Chem.*, Heidelb., DE, 10.10
2018 Invited speaker *Computational Catalysis for Sustainable Chemistry*, Spain, 13-15.6.

ORGANISATION OF SCIENTIFIC MEETINGS

2019 Member of local organizing committee for *ISTCP-X*, Norway (~550 participants)
2019 Co-organizer of full day session as part of *EuCOMC 2019*, Finland (~220 participants)
2018 Organizer of *1st meeting of the Nordic Consortium for CO_2 Conversion*, UiT, 31 participants
2015 Co-organizer of *Numerical Methods in Quantum Chemistry*, Norway, ~60 participants

MAJOR COLLABORATORS

2017 – Prof. **Timo Repo**, Helsinki University, Finland.
2016 – Prof. **Paul Chirik**, Princeton University, USA.
2010 – Assoc. Prof. **Annette Bayer**, Dept. Chemistry, UiT.
2010 – 2013 Prof. **Petr Bour**, Institute of Organic Chemistry and Biochemistry, Prague, Czech Republic.
2009 – 2016 Prof. **Louis Noodleman**, Scripps Research Institute, USA.
2009 – 2015 Prof. **Jeanet Conradie**, Dept. of Phys. Chem., University of the Free State, South Africa.

SUMMARY OF PUBLICATIONS

• I have co-authored **54 peer-reviewed scientific articles** in international journals, 3 peer-reviewed book chapters, 4 editorials and several comments. My **h-index is 26**, with ~2000 citations (Google Scholar).

• Of my 57 peer-reviewed articles & chapters, 47 are from the ~11 years of active research since my PhD award, **29 are as 1st author, 23 as corresponding,** and **16 as last or single author.**

PUBLICATION LIST

Peer-reviewed Scientific Articles *(*marks all corresponding authors, [OA]marks open access publications)*

1) [OA]**Multiwavelets Applied to Metal-Ligand Interactions: Energies Free from Basis Set Errors. ChemRxiv** Brakestad, A.; Wind, P.; Jensen, S. Rune; Frediani, L.*; Hopmann, KH* *ChemRxiv* **2021**, *Preprint.*
2) [OA]**Computational and experimental insights into asymmetric Rh-catalyzed hydrocarboxylation with CO_2** Pavlovic, Lj; Pettersen, M; Gevorgyan, A; Vaitla, J; Bayer, A*, Hopmann, KH*; *Eur. J. Org. Chem.* **2020**, 663.
3) [OA]**Ni(I)-Alkyl Complexes Bearing Phenanthroline Ligands: Experimental Evidence for CO_2 Insertion at Ni(I) Centers**, Somerville, RJ; Odena, O; Obst, MF; Hazari, N; Hopmann, KH*; Martin, R*, *JACS* **2020**, *142*, 10936. ***OA*** in *ChemRxiv*.
4) [OA]**Static polarizabilities at the basis set limit: A benchmark of 124 species**, Brakestad, A; Jensen, SR, Wind, P; D'Alessandro, M; Genovese, L.; Hopmann, KH; Frediani, L*, *J. Chem. Theory Comp.* **2020**, *16*, 4874.
5) **Mechanistic insights into copper-catalyzed carboxylations**, Obst, M; Gevorgyan, A; Bayer, A*; Hopmann, KH* *Organometallics* **2020**, *39*, 1545. *Part of Special Issue, which I edited and designed the cover for.*
6) [OA]**To bind or not to bind: Mechanistic insights into C–CO_2 bond formation with late transition metals**, García-López, D; Pavlovic, Lj; Hopmann, KH*, *Organometallics* **2020**, *39*, 1339.
7) [OA]**Formal C-H Carboxylation of Unactivated Arenes**, Gevorgyan, A*; Hopmann, KH; Bayer, A*, *Chem. Eur. J.* **2020**, *26*, 6064.
8) [OA]**Exploration of New Biomass-Derived Solvents: Application to Carboxylation Reactions**, Gevorgyan, A*; Hopmann, KH; Bayer, A* *ChemSusChem* **2020**, *13*, 2080.
9) [OA]**Caesium Fluoride-Mediated Hydrocarboxylation of Alkenes and Allenes: Scope and Mechanistic Insights** Gevorgyan, A; Obst, M; Guttormsen, Y; Maseras, F; Hopmann, KH*; Bayer, A*; *Chemical Science* **2019**, *10*, 10072.
10) **Vinyl Sulfoxonium Ylide: A New Vinyl Carbenoid Transfer Reagent for the Synthesis of Heterocycles** Vaitla, J*; Bayer, A; Hopmann, KH*; *Synlett* **2019**, *30*, 1377.
11) **Iron-Catalyzed Carbenoid Transfer Reactions of Vinyl Sulfoxonium Ylides: An Experimental and Computational Study**, Vaitla, J*; Bayer, A; Hopmann, KH*, *Angew. Chem. IE* **2018**, *57*, 16180.
12) [OA]**Cobalt-Catalysed Alkene Hydrogenation: A Metallacycle Can Explain the Hydroxyl Activating Effect and the Diastereoselectivity** Morello, GR; Zhong, H; Chirik, PJ; Hopmann, KH*; *Chemical Science* **2018**, ***9***, 4977.
13) **Rhodium-Catalyzed Hydrocarboxylation: Mechanistic Analysis Reveals Unusual Transition State for C-C Bond Formation** Pavlovic, L; Vaitla, J; Bayer, A; Hopmann, KH*; *Organometallics* **2018**, *37*, 941.
14) [OA]**Carbon-Carbon bonds with CO_2: Insights from Computational Studies** Obst, M; Pavlovic, Lj; Hopmann, KH*; *J. Organomet. Chem.* **2018**, *864*, 115. (*Invited mini-review*)
15) **Rhodium-Catalyzed Synthesis of Sulfur Ylides via in Situ Generated Iodonium Ylides** Vaitla, J*; Hopmann, KH, Bayer, A; *Organic Letters* **2017**, *19*, 6688.
16) **Enantioselective CO_2 Incorporation: Status and Potential** Vaitla, J; Guttormsen, Y; Mannisto, J; Nova, A; Repo, T; Bayer, A*; Hopmann, KH*; *ACS Catalysis* **2017**, *7*, 7231 (*Invited Perspective article*)
17) **A Dihydride Mechanism Can Explain the Intriguing Substrate Selectivity of Iron-PNP-Mediated Hydrogenation** Morello, G; Hopmann, KH*; *ACS Catalysis* **2017**, *7*, 5847
18) **Synthesis of Indoles and Pyrroles Utilizing Iridium Carbenes Generated from Sulfoxonium Ylides**, Vaitla, J*; Bayer, A; Hopmann, KH; *Angewandte Chemie, International Edition* **2017**, *56*, 4277.
19) [OA]**How accurate is DFT for iridium-mediated chemistry** Hopmann, KH*; *Organomet.* **2016, *35*, 3795.** *(Featured on cover)*
20) **Structure, substitution and hydrolysis of bis(trifluorobenzoylacetonato-O,O')dichloro Ti(IV): an experimental and computational study** Kuhn, A; Tischlik, S; Hopmann, KH; Landman, M; van Royen, P; Conradie, J*; *Inorg. Chim. Acta* **2016,** *453*, 345.
21) **Computer Simulations Reveal Substrate Specificity of Glycosidic Bond Cleavage in Native and Mutant Human Purine Nucleoside Phosphorylase,** Isaksen, G. V; Hopmann, KH; Åqvist, J; Brandsdal, BO*; *Biochemistry* **2016**, *55*, 2153.
22) **Singlet–Triplet Gaps of Cobalt Nitrosyls: Insights from Tropocoronand Complexes,** Hopmann, KH; Conradie, J; Tangen, E; Tonzetich, ZJ; Lippard, SJ; Ghosh, A*; *Inorg. Chem.* **2015**, *54*, 7362.
23) **Iron-Brønsted-acid-catalysed asymmetric hydrogenation: Mechanism and selectivity-determining interactions**, Hopmann, KH*; *Chem. Eur. J.* **2015**, *21*, 10020. (*Featured as* Frontispiece *that I designed).*
24) [OA]**Quantum chemical studies of asymmetric reactions: Historical aspects and recent examples**, Hopmann, KH*; *Inter. J. Quant. Chem.* **2015**, *115*, 1232. *(Invited review)*
25) **Iridium-PHOX-mediated alkene hydrogenation: Isomerisation influences the stereochemical outcome**, Hopmann, KH*; Frediani, L, Bayer, A. *Organometallics*, **2014**, 33, 2790.
26) **Full reaction mechanism of nitrile hydratase: a cyclic intermediate and an unexpected disulfide switch,** Hopmann, KH*; *Inorg. Chem.*, **2014**, *53*, 2760. (*Communication*)
27) **Enantioselective Imine Hydrogenation with iridium Catalysts: Reactions, Mechanisms, and Stereocontrol,** Hopmann, KH*; Bayer, A *Coord. Chem. Rev.* **2014**, *268*, 59. (*Review*)
28) **Substitution kinetics of aryl diolato ligands at dichlorobis(betadiketonato-*O,O'*)titanium (IV): Experimental and Computational study.** Hopmann, KH; Kuhn, A; Conradie, J*; *Polyhedron* **2014**, *67*, 231.

29) **Cobalt-Bis(imino)pyridine-Catalyzed Asymmetric Hydrogenation: Electronic Structure, Mechanism, and Stereoselectivity,** Hopmann, KH*; *Organometallics* **2013**, *32*, 6388.
30) **Determination of Absolute Configuration and Conformation of a Cyclic Dipeptide by NMR and Chiral Spectroscopic Methods,** Li, X.-J; Hopmann, KH*; Hudecova, J; Isaksson, J; Novotna, J; Stensen, W; Andrushchenko, V; Urbanova, M; Svendsen, JS; Bour, P*; Ruud, K; *J. Phys. Chem. A*, **2013**, *117*, 1721.
31) **Circular Dichroism and Optical Rotation of Lactamide and 2-Aminopropanol in Aqueous Solution,** Pikulska, A; Hopmann, KH; Bloino, J; Pecul, M*; *J. Phys. Chem. B* **2013**, 117, 5136.
32) **Correction of the Vibrational Broadening in Molecular Dynamics Clusters with the Normal Mode Optimization Method,** Hudecova, J ; Hopmann, KH; Bouř, P*; *J. Phys. Chem. B.* **2012**, *116*, 336.
33) **Absolute configuration of a cyclic dipeptide reflected in vibrational optical activity: *ab initio* and experimental investigation,** Li, X; Hopmann, KH; Hudecova, J; Stensen, W; Novotná, J; Urbanová, M; Svendsen, J; Bouř, P*; Ruud, K* *JPC A* **2012**, *116*, 2554.
34) **Determining the absolute configuration of two marine compounds using vibrational vhiroptical spectroscopy** Hopmann, KH*; Šebestík, J; Novotná, J; Stensen, W; Urbanová, M; Svenson, J; Svendsen, JS; Bouř, P*; Ruud, K; *JOC* **2012**, *77*, 858.
35) **Mechanism of Cobalt-Porphyrin-Catalyzed Aziridination,** Hopmann, KH; Ghosh, A*; *ACS Catalysis* **2011**, *1*, 597.
36) **Calibration of DFT Functionals for the Prediction of ^{57}Fe Mössbauer Spectral Parameters in Iron-Nitrosyl and Iron-Sulfur Complexes.** Sandala, GM; Hopmann, KH; Ghosh, A; Noodleman, L*; *J. Chem. Theory. Comp.* **2011**, *7*, 3232.
37) **Hemoglobin as Nitrite Anhydrase: Modeling Methemoglobin-Mediated N_2O_3 Formation,** Hopmann, KH; Cardey, B; Gladwin, MT; Kim-Shapiro, DB; Ghosh, A*; *Chem. Eur. J.* **2011**, *17*, 6348 *(Article featured on the Cover)*
38) **Explicit versus Implicit Solvent Modeling of Raman Optical Activity Spectra,** Hopmann, KH*; Ruud, K; Pecul, M; Kudelski, A; Dračínský, M; Bouř, P*; *J. Phys. Chem. B.* **2011,** *115*, 4128.
39) **On the Mechanism of Iridium-Catalysed Asymmetric Hydrogenation of Imines and Alkenes: A Theoretical Study,** Hopmann, KH*; Bayer, A; *Organometallics* **2011**,*30*, 2483.
40) **Spin Coupling in Roussin's Red and Black Salts,** Hopmann, KH; Noodleman, L*; Ghosh, A*; *Chem. Eur. J.* **2010**, *16*, 10397.
41) **Understanding the Unusually Straight: A Search for MO Insights into Linear {FeNO}^{7} Units,** Conradie, J; Hopmann, KH; Ghosh, A*; *J. Phys. Chem. B* **2010**, *114*, 8517.
42) **Substitution and Isomerisation of Asymmetric β-Diketonato Rhodium(I) Complexes: A Crystallographic and Computational Study,** Hopmann, KH; Stuurman, NF; Muller, A; Conradie, J*; *Organometallics* **2010**, *29*, 2446.
43) **Density Functional Theory Calculations on Mössbauer Parameters of Nonheme Iron Nitrosyls,** Hopmann, KH; Ghosh, A*; Noodleman, L*; *Inorg. Chem.* **2009**, *48*, 9155.
44) **Broken-Symmetry DFT Spin Densities of Iron Nitrosyls, Including Roussin's Red and Black Salts: Striking Differences between Pure and Hybrid Functionals,** Hopmann, KH; Conradie, J; Ghosh, A*; *J. Phys. Chem. B* **2009**, *113*, 10540.
45) **Density Functional Theory Study of Substitution at the Square-Planar Acetylacetonato-dicarbonyl-rhodium(I) Complex,** Hopmann, KH; Conradie, J; *Organometallics* **2009**, *28*, 3710.
46) **On the Role of Tyrosine as Catalytic Base in Nitrile Hydratase,** Hopmann, KH; Himo, F*, *Eur. J. Inorg. Chem.* **2008**, 3452.
47) **Quantum chemical modeling of the dehalogenation reaction of haloalcohol dehalogenase**, Hopmann, KH; Himo, F; *J. Chem. Theory Comp.* **2008**, *4*, 1129.
48) **Cyanolysis and Azidolysis of Epoxides by Haloalcohol Dehalogenase: Theoretical Study of the Reaction Mechanism and Origins of Regioselectivity,** Hopmann, KH; Himo, F; *Biochemistry* **2008**, *47*, 4973.
49) **Theoretical investigation of the second-shell mechanism of nitrile hydratase,** Hopmann, KH; Himo, F*; *EJIC* **2008**, *9*, 1406.
50) **Theoretical investigation of the first-shell mechanism of nitrile hydratase,** Hopmann, KH; Guo, JD; Himo, F*; *Inorg. Chem.* **2007**, *46*, 4850.
51) **Efficient Expression of Recombinant Human Monoclonal Antibodies in Drosophila S2 cells,** Johansson, DX; Drakenberg, K; Hopmann, KH; Schmidt, A; Yari, F; Hinkula, J; Persson, MA*; *J. Immunol. Methods.* **2007**, *318*, 37.
52) **Insights into the reaction mechanism of soluble epoxide hydrolase from theoretical active site mutants**, Hopmann, KH; Himo, F*; *J. Phys. Chem. B.* **2006,** *110*, 21299.
53) **Theoretical study of the Full Reaction Mechanism of Human Soluble Epoxide Hydrolase,** Hopmann, KH; Himo, F*; *Chem. Eur. J.* **2006**, *12*, 6898.
54) **Catalytic Mechanism of Limonene Epoxide Hydrolase, a Theoretical Study,** Hopmann, KH; Hallberg, BM; Himo, F*; *J. Am. Chem. Soc.* **2005**, *127*, 14339.
55) **Substrate specificity of the metalloproteinase pregnancy-associated plasma protein-A assessed by mutagenesis and analysis of synthetic peptides: substrate residues distant from the scissile bond are critical for proteolysis,** Laursen, LS; Overgaard, M; Nielsen, CG, Boldt, HB; Hopmann, KH; Conover, CA; Sottrup-Jensen, L; Giudice, LC; Oxvig, C*; *Biochem. J.* **2002**, *367*, 31.

Book Chapters and Theses

56) **Electronic structure, bonding, spin coupling & energetics of polynuclear iron sulfur clusters-a broken symmetry DFT perspective** Hopmann, KH; Pelmenschikov, V; Handu, W; Noodleman, L *Spin states in Biochem.&Inorg.Chem.* Ed Swart, Wiley **2015**, 297.
57) **Quantum Chemical Modeling of Enzymatic Reactions – Applications to Epoxide-Transforming Enzymes,** Hopmann, KH; Himo, F. in *Comprehensive Natural Products II, Chemistry and Biology;* Eds. Mander, L; Lui, HW; **2010**; vol. 8, 719.
58) **Electronic Structure Calculations: Transition Metal-NO Complexes** Ghosh, A; Hopmann, KH; Conradie, J; in *Computational Inorganic and Bioinorganic Chemistry*; Eds. Solomon, EI, Scott, RA, King, RB; **2009**; pp 389.
59) **Nitrile Hydratases and Epoxide-Transforming Enzymes: Quantum Chemical Modeling of Reaction Mechanisms and Selectivities,** Hopmann, KH, PhD Thesis, KTH Stockholm, Sweden **2008.**
60) **Quantum chemical studies of epoxide-transforming enzymes,** Hopmann, KH, Licentiate thesis, KTH **2007**

Editorials, Popular Science Articles, Comments

61) **Annual Report 2019 Nordic Consortium For CO_2 Conversion** Hopmann, KH with contributions from others, **2020**.

62) **A Polymer Magician: Prof. Charlotte K. Williams** Hopmann, KH*, *Organometallics* **2020**, *39*, 3291.
63) **Handlingsplan for Ulikestilling og Ekskludering**, Hopmann, KH*, *Khrono*, 24.02.**2020**.
64) **Organometallic chemistry for enabling CO_2 utilization** Hazari, N; Iwasawa, N; Hopmann, KH*, *Organometallics* **2020**, *39*, 1457
65) **Annual Report 2018 Nordic Consortium For CO_2 Conversion** Hopmann, KH with contributions from others, **2019**.
66) **How To Make Your Computational Paper Interesting and Have It Published** Hopman, KH* *Organometallics* **2019**, *38*, 603.
67) **Trodde Du?** Dundas, K. O. H; Hopmann, KH; Olsson, M. *NordNorsk Debatt*, 28.09.**2018**.
68) **Hvordan kan UiT's restrukturering gjøres mer hensiktsmessig?** Frediani, L; Hopmann, KH; *et al NordNorskDebatt*, 21.6.**2017**
69) **FemEx—Female excellence in theoretical and computational chemistry** Mennucci, B; Eisenstein, O; Fliegl, H; Hopmann, KH; Helgaker, T; Ruud, K; *Int. J. Quantum Chem.* **2015**, *115*, 1195–1196.
70) **Project CHOCO: Catalysts for CO_2 Conversion** Hopmann, KH*; **2017**, in "*CTCC annual report 2016"*.
71) **The new ABC of chemistry: Asymmetric Base-metal Catalysis** Hopmann, KH*; **2014** in **"***CTCC annual report 2013***"**.
72) **Kiroptisk spektroskopi** Hopmann, KH; Ruud, K; *Kjemi* **2011**
73) **Datamaskiner beregner verden** Hopmann, KH; Ruud, K; *Nordlys* 27.09.**2010**