

Curriculum Vitae

Personal Information

Full Name Nina Strasser
Date of Birth June 27th, 1998
Place of Birth Graz, Austria
Citizenship Austria
Gender Female
Email nina.strasser@rub.de
External links  ORCID  Google Scholar  ResearchGate
 LinkedIn  Web of Science



Research Interests

- Vibrational and phonon properties of metal-organic frameworks
- Thermal expansion and mechanical properties of crystalline solids
- Machine-learned interatomic potentials for solid state systems
- Structure-to-property relationships studied by first-principles simulations
- Solvation effects with spectroelectrochemistry

Employment

2025–Present **Postdoctoral Researcher (Solvation Science)**
Group of Prof. Martina Havenith-Newen at Ruhr-University Bochum

2022–2025 **Doctoral Researcher (Solid State Physics)**
Group of Prof. Egbert Zojer at Graz University of Technology

2020–2022 **Pre-Doctoral Researcher (Physical and Theoretical Chemistry)**
Group of Prof. A. Daniel Boese at the University of Graz

2018–2020 **Research Assistant (Theoretical Chemistry)**
Group of Ao.Univ-Prof.i.R. Alexander Sax at University of Graz

2017–2018 **Research Assistant (Computational Chemistry)**
Group of Ao.Univ.-Prof. Anne-Marie Kelterer at Graz University of Technology

Education

2022–2025 **PhD in Natural Sciences (Dr.rer.nat.)**
Graz University of Technology
Summa cum laude (Grade: 1.0 / Excellent)

2019–2020 **Master of Science in Chemistry (MSc)**
Graz University of Technology and University of Graz (NAWI Graz Cooperation)
Graduated with Distinction

2016–2019 **Bachelor of Science in Chemistry (BSc)**
Graz University of Technology and University of Graz (NAWI Graz Cooperation)

Publications

Papers in Peer-Reviewed Journals

- **From Monolayer to Bulk: Thin-Film-Specific Polymorphic Transitions of a Molecular Semiconductor**
Nobutaka Shioya, Fabian Gasser, Nina Strasser, Egbert Zojer, Roland Resel, Josef Simbrunner and Takeshi Hasegawa, *Chemistry of Materials*, (2026).
- **Insights into phonons and spinlattice relaxation in copper(II) and vanadyl(IV) porphyrin metalorganic frameworks from density functional theory**
Yukina Suzuki, Nina Strasser, Ryota Sakamoto and Masahiro Yamashita, *Phys. Chem. Chem. Phys.*, 28, 2858-2872 (2026).
- **Influence of pore-confined water on the thermal expansion of a zinc-based metal-organic framework**
Nina Strasser, Benedikt Schrode, Ana Torvisco, Sanjay John, Birgit Kunert, Brigitte Bitschnau, Florian P. Lindner, Christian Slugovc, Egbert Zojer and Roland Resel, *Journal of Materials Chemistry C*, 33, 17353-17366 (2025).
- **Identifying Structure and Texture of Metal-Organic Framework Thin Films by Combining X-ray Diffraction and Quantum Mechanical Modelling**
Mario Fratschko, Nina Strasser, Narges Taghizade, Mercedes Linares-Moreau, Jan C. Fischer, Tonghan Zhao, Ian A. Howard, Paolo Falcaro, Egbert Zojer and Roland Resel, *Crystal Growth and Design*, 25 (11), 3665-3679 (2025).
- **Chemical Bonding in Three-Membered Ring Systems**
Nina Strasser and Alexander F. Sax, *Molecules*, 30 (3), 612 (2025).
- **Combining Brillouin spectroscopy and machine learned interatomic potentials to probe mechanical properties of metal organic frameworks**
Florian P. Lindner, Nina Strasser, Martin Schultze, Sandro Wieser, Christian Slugovc, Kareem Elsayad, Kristie J. Koski, Egbert Zojer and Caterina Czibula, *The Journal of Physical Chemistry Letters*, 16 (5), 1213-1220 (2025).

○ **The Seventh Blind Test of Crystal Structure Prediction:
Structure Generation Methods**

Lily M. Hunnisett, Jonas Nyman, Nicholas Francia, Nathan S. Abraham, Claire S. Adjiman, Srinivasulu Aitipamula, Tamador Alkhidir, Mubarak Almehairbi, Andrea Anelli, Dylan M. Anstine, John E. Anthony, Joseph E. Arnold, Faezeh Bahrami, Michael A. Bellucci, Rajni M. Bhardwaj, Imanuel Bier, Joanna A. Bis, A. Daniel Boese, David H. Bowskill, James Bramley, Jan Gerit Brandenburg, Doris E. Braun, Patrick W. V. Butler, Joseph Cadden, Stephen Carino, Eric J. Chan, Chao Chang, Bingqing Cheng, Sarah M. Clarke, Simon J. Coles, Richard I. Cooper, Ricky Couch, Ramon Cuadrado, Tom Darden, Graeme M. Day, Hanno Dietrich, Yiming Ding, Antonio DiPasquale, Bhausahab Dhokale, Bouke P. van Eijck, Mark R. J. Elsegood, Dzmitry Firaha, Wenbo Fu, Kaori Fukuzawa, Joseph Glover, Hitoshi Goto, Chandler Greenwell, Rui Guo, J Hartergen, Julian Helfferich, Detlef W. M. Hofmann, Johannes Hoja, John Hone, Richard Hong, Geoffrey Hutchison, Yasuhiro Iwabata, Olexandr Isayev, Ommair Ishaque, Varsha Jain, Yingdi Jin, Aling Jing, Erin R. Johnson, Ian Jones, K. V. Jovan Jose, Elena A. Kabova, Adam Keates, Paul F. Kelly, Dmitry Khakimov, Stefanos Konstantinopoulos, Liudmila N. Kuleshova, He Li, Xiaolu Lin, Alexander List, Congcong Liu, Yifei Michelle Liu, Zenghui Liu, Zhi-Pan Liu, Joseph W. Lubach, Noa Marom, Alexander A. Maryewski, Hiroyuki Matsui, Alessandra Mattei, R. Alex Mayo, John W. Melkumov, Sharmarke Mohamed, Zahrasadat Momenzadeh Abardeh, Hari S. Muddana, Naofumi Nakayama, Kamal Singh Nayal, Marcus A. Neumann, Rahul Nikhar, Shigeaki Obata, Oana Connor, Artem R. Oganov, Koji Okuwaki, Alberto Otero-de-la-Roza, Constantinos C. Pantelides, Sean Parkin, Chris J. Pickard, Luca Pilia, Tatyana Pivina, Rafal Podeszwa, Alastair J. A. Price, Louise S. Price, Sarah L. Price, Michael R. Probert, Angeles Pulido, Gunjan Rajendra Ramteke, Atta Ur Rehman, Susan M. Reutzel-Edens, Jutta Rogal, Marta J. Ross, Adrian F. Rumson, Ghazala Sadiq, Zeinab M. Saeed, Alireza Salimi, Matteo Salvalaglio, Leticia Sanders de Almada, Kiran Sasikumar, Sivakumar Sekharan, Cheng Shang, Kenneth Shankland, Kotaro Shinohara, Baimei Shi, Xuekun Shi, A. Geoffrey Skillman, Hongxing Song, Nina Strasser, Jacco van de Streek, Isaac J. Sugden, Guangxu Sun, Krzysztof Szalewicz, Benjamin I. Tan, Lu Tan, Frank Tarczynski, Christopher R. Taylor, Alexandre Tkatchenko, Rithwik Tom, Mark E. Tuckerman, Yohei Utsumi, Leslie Vogt-Maranto, Jake Weatherston, Luke A. Wilkinson, Robert D. Willacy, Lukasz Wojtas, Grahame R. Woollam, Zhuocen Yang, Etsuo Yonemochi, Xin Yue, Qun Zeng, Yizu Zhang, Tian Zhou, Yunfei Zhou, Roman Zubatyuk and Jason C. Cole, *Structural Science*, 80 (6) (2024).

- **The Seventh Blind Test of Crystal Structure Prediction: Structure Ranking Methods**

Lily M. Hunnisett, Nicholas Francia, Jonas Nyman, Nathan S. Abraham, Srinivasulu Aitipamula, Tamador Alkhidir, Mubarak Almehairbi, Andrea Anelli, Dylan M. Anstine, John E. Anthony, Joseph E. Arnold, Faezeh Bahrami, Michael A. Bellucci, Gregory J. O. Beran, Rajni M. Bhardwaj, Raffaello Bianco, Joanna A. Bis, A. Daniel Boese, James Bramley, Doris E. Braun, Patrick W. V. Butler, Joseph Cadden, Stephen Carino, Ctirad Cervinka, Eric J. Chan, Chao Chang, Sarah M. Clarke, Simon J. Coles, Cameron J. Cook, Richard I. Cooper, Tom Darden, Graeme M. Day, Wenda Deng, Hanno Dietrich, Antonio DiPasquale, Bhausahab Dhokale, Bouke P. van Eijck, Mark R. J. Elsegood, Dzmitry Firaha, Wenbo Fu, Kaori Fukuzawa, Nikolaos Galanakis, Hitoshi Goto, Chandler Greenwell, Rui Guo, J Hartergen, Julian Helfferich, Johannes Hoja, John Hone, Richard Hong, Michal Husak, Yasuhiro Iwabata, Olexandr Isayev, Ommair Ishaque, Varsha Jain, Yingdi Jin, Aling Jing, Erin R. Johnson, Ian Jones, K. V. Jovan Jose, Elena A. Kabova, Adam Keates, Paul F. Kelly, Jiri Klimes, Veronika Kostkova, He Li, Xiaolu Lin, Alexander List, Congcong Liu, Yifei Michelle Liu, Zenghui Liu, Ivor Loncaric, Joseph W. Lubach, Jan Ludik, Alexander A. Maryewski, Noa Marom, Hiroyuki Matsui, Alessandra Mattei, R. Alex Mayo, John W. Melkumov, Bruno Mladineo, Sharmarke Mohamed, Zahrasadat Momenzadeh Abardeh, Hari S. Muddana, Naofumi Nakayama, Kamal Singh Nayal, Marcus A. Neumann, Rahul Nikhar, Shigeaki Obata, Oana Connor, Artem R. Oganov, Koji Okuwaki, Alberto Otero-de-la-Roza, Sean Parkin, Antonio Parunov, Rafal Podeszwa, Alastair J. A. Price, Louise S. Price, Sarah L. Price, Michael R. Probert, Angeles ulido, Gunjan Rajendra Ramteke, Atta Ur Rehman, Susan M. Reutzel-Edens, Jutta Rogal, Marta J. Ross, Adrian F. Rumson, Ghazala Sadiq, Zeinab M. Saeed, Alireza Salimi, Kiran Sasikumar, Sivakumar Sekharan, Kenneth Shankland, Baimei Shi, Xuekun Shi, Kotaro Shinohara, A. Geoffrey Skillman, Hongxing Song, Nina Strasser, Jacco van de Streek, Isaac J. Sugden, Guangxu Sun, Krzysztof Szalewicz, Lu Tan, Kehan Tang, Frank Tarczyski, Christopher R. Taylor, Alexandre Tkatchenko, Petr Tous, Mark E. Tuckerman, Pablo A. Unzueta, Yohei Utsumi, Leslie Vogt-Maranto, Jake Weatherston, Luke A. Wilkinson, Robert D. Willacy, Lukasz Wojtas, Grahame R. Woollam, Yi Yang, Zhuocen Yang, Etsuo Yonemochi, Xin Yue, Qun Zeng, Tian Zhou, Yunfei Zhou, Roman Zubatyuk and Jason C. Cole, *Structural Science*, 80 (6) (2024).

- **Predicting Spin-Dependent Phonon Band Structures of HKUST-1 Using Density Functional Theory and Machine-Learned Interatomic Potentials**
Nina Strasser, Sandro Wieser and Egbert Zojer, *International Journal of Molecular Sciences*, 25 (5), 3023 (2024).

- **Competing Intramolecular Hydrogen Bond Strength and Intermolecular Interactions in the 4-Aminobutanol–Water Complex**
Jenna Hohl, Michael Harris, Nina Strasser, Anne-Marie Kelterer and Richard Lavrich, *The Journal of Physical Chemistry A*, 122 (43), 8505-8510 (2018).

Doctoral Thesis

- Title **Structure and Phonon Properties of Metal-Organic Frameworks**
- Supervisor Univ-Prof. Egbert Zojer
- Co-supervisor Ao.-Univ-Prof. Roland Resel
- Institute Solid State Physics at Graz University of Technology, Austria
- Content My PhD research focused on the vibrational properties of metal-organic frameworks (MOFs) and their relationship to key material characteristics such as thermal expansion, mechanical stability and magnetic behavior. I investigated spin-dependent phonon band structures in the MOF HKUST-1 using both density functional theory and machine-learned moment tensor potentials. In a second case study, I studied the impact of pore-confined water molecules on the thermal expansion coefficients in the MOF GUT-2 through temperature-dependent X-ray diffraction. Finally, I demonstrated how simulated IR spectra can support the structural characterization of MOF thin films and molecular crystals.

Master Thesis

- Title **Reactions of Three-Ring Molecules and Molecules with Multiple Bonds: An OVB Analysis (Orthogonal Valence Bond)**
- Supervisor Ao.Univ-Prof.i.R. Alexander Sax
- Institute Physical and Theoretical Chemistry at University of Graz, Austria
- Content In this master thesis, a recently developed OVB method is used to investigate the dissociation of a triple bond and of a double bond as well as the elimination of carbene and silylene from four three-ring molecules and the respective reverse reactions. Local effects are usually hidden by wave functions that are constructed with delocalized orbitals. OVB wave functions are built with orthogonal localized orbitals and are able to describe local spin and charge redistributions.

Bachelor Thesis

- Title **A Computational Study of Hydrogen Bonding in the System 3-Aminopropanol–Water**
- Supervisor Ao.Univ.-Prof. Anne-Marie Kelterer
- Institute Physical and Theoretical Chemistry at Graz University of Technology, Austria
- Content This bachelor thesis is a theoretical study about dimers of the amino-alcohol 3-aminopropanol and their clusters including water. It answers the question which types of hydrogen bonds can be formed and how they have an impact on the stabilization of molecular clusters. Moreover, it investigates which spectroscopic methods are suitable to distinguish between different clusters.

Awards and Funding

- 2024 **Competitive Initial Funding (€ 6000)**
Field of Expertise Advanced Material Science
University of Technology, Graz
- 2020 **Merit-based Scholarship in Chemistry (Master Study Programme)**
Faculty of Technical Chemistry, Chemical and Process Engineering
University of Technology, Graz
- 2018 **Merit-based Scholarship in Chemistry (Bachelor Study Programme)**
Faculty of Technical Chemistry, Chemical and Process Engineering
University of Technology, Graz

Scientific Presentations

Invited Talks

- **Simulating Porous Materials: Spins, Phonons and Water**
Nina Strasser, *Ruhr-University Bochum*, Bochum (Germany), 2025

Oral Presentations

- **Predicting Spin-Dependent Phonon Band Structures of HKUST-1 with Machine-Learned Interatomic Potentials**
Nina Strasser, Benedikt Schrode, Ana Torvisco Gomez, Sanjay John, Katharina Kodolitsch, Christian Slugovc, Egbert Zojer and Roland Resel, *20th Austrian Chemistry Days*, Graz (Austria), 2024
- **Influence of Pore-Confined Water on the Thermal Expansion of a Zinc-Based Metal-Organic Framework**
Nina Strasser, Benedikt Schrode, Ana Torvisco Gomez, Sanjay John, Katharina Kodolitsch, Christian Slugovc, Egbert Zojer and Roland Resel, *XRD excites: Non-Ambient XRD & Beyond, International XRD Symposium 2024*, Graz (Austria), 2024 | **NON-AMBIENT XRD PHOTO AWARD**
- **Predicting Spin-Dependent Phonon Band Structures of HKUST-1 with Machine-Learned Interatomic Potentials**
Nina Strasser, Sandro Wieser and Egbert Zojer, *Workshop Machine Learning for Chemistry*, Bad Hofgastein (Austria), 2024
- **Hydrogen Bonding in the System 3-Aminopropanol–Water**
Nina Strasser, *4th Polish-Taiwanese Conference*, Opole (Poland), 2018 | **AWARD FOR THE BEST YOUNG SCIENTIST LECTURE**

Poster Presentations

- **Influence of pore-confined water and hydration state on thermal expansion of a zinc-based metal-organic framework**
Nina Strasser, Benedikt Schrode, Ana Torvisco Gomez, Sanjay John, Katharina Kodolitsch, Brigitte Bitschnau, Florian Patrick Lindner, Christian Slugovc, Egbert Zojer and Roland Resel, *6th European Conference on Metal Organic Frameworks and Porous Polymers (EUROMOF2025)*, Heraklion (Greek), 2025

- **Influence of pore-confined water and hydration state on thermal expansion of a zinc-based metal-organic framework**
Nina Strasser, Benedikt Schrode, Ana Torvisco Gomez, Sanjay John, Katharina Kodolitsch, Brigitte Bitschnau, Florian Patrick Lindner, Christian Slugovc, Egbert Zojer and Roland Resel, *Conference on Biotechnological and Biomedical Applications of Porous Materials (BBPore)*, Graz (Austria), 2025
- **How accurate can machine-learned force fields describe spin-polarized dependent vibrations of HKUST-1 compared to density functional theory?**
Nina Strasser, Narjes Taghizadeh Rahaghi, Sandro Wieser, Lukas Legenstein and Egbert Zojer, *5th European Conference on Metal Organic Frameworks and Porous Polymers: EUROMOF2023*, Granada (Spain), 2023
- **Applying the Stochastic Self-Consistent Harmonic Approximation to Metal-Organic Frameworks**
Nina Strasser, Francesco Carraro, Roman Lucrezi, Sandro Wieser, Paolo Falcaro and Egbert Zojer, *Finite-temperature and anharmonic response properties of solids in theory and practice: TDEP Workshop*, Linköping (Sweden), 2023
- **Evaluation of a Novel Schiff Base Polypyrrole Actuator - a DFT and FTIR Study**
Nina Strasser and Anne-Marie Kelterer, *Interfacing Machine Learning and Experimental Methods for Surface Structures*, Graz (Austria), 2018

Teaching Experience

Ruhr University Bochum, Germany

- **Physical Foundations of Chemistry** (Physikalische Grundlagen der Chemie)
 Winter term 2025/26 [F2F]

Graz University of Technology, Austria

- **Physics for Electrical Engineering** (Physik (ET))
 Winter terms 2023/24, 2024/25 [F2F]

University of Graz, Austria

- **Physical Chemistry Lab Course** (LU aus Physikalischer Chemie)
 Winter term 2021/22 [online]
- **Molecular Analytics and Spectroscopy Lab Course** (LU aus Molekularer Analytik und Spektroskopie)
 Winter term 2021/22 [hybrid]
- **Mathematics for Chemists II** (Mathematik für ChemikerInnen II)
 Summer term 2020/21 [online]
- **Calculus of Physical Chemistry II** (Rechenübungen aus Physikalischer Chemie II)
 Winter term 2020/21 [online]

Supervision

- **Bachelors theses:** 1 co-supervised (Graz University of Technology, Institute of Solid State Physics, 2025)

Academic Service

- Co-organizer of the Doctoral Days Chemistry 2025 (DocDays 2025), NAWI Graz, Austria.
- Co-organizer of the 3rd PhD Symposium of the PMWS project, Graz University of Technology, Austria.
- Peer reviewer for the international peer-reviewed journal *Chemical Monthly*.

Trainings and Certificates

- Young Leaders Programme (2024)
- High Potential Coaching (2024)
- Project Management Compact (2024)
- Time Management 2: Techniques for Planning and Scheduling (2023)
- Time Management 1: Fundamentals (2023)
- Sexual Harassment and Sexualized Violence: Intervention Options, Legal Framework and Responsibilities for People in Leadership Positions (2023)
- Rhetoric for Conversations and Meetings: Argumentation, Communication Techniques, Moderation (2023)
- Conflicts in the Workplace: Challenges and Opportunities (2022)

Languages

German Mother Tongue
English C1 Level

Skills and Software

Programming Bash, C, Fortran, Python
Simulation VASP, FHI-aims, CRYSTAL23, Phonopy, MLIP, Gaussian, Orca, Turbomole
Visualization VESTA, Mercury, Avogadro, Ovito