

RESOLV 2019-2025: SCIENTISTS

PRINCIPAL INVESTIGATORS

PERSON	RESEARCH FIELDS
 Prof. Dr. Uwe Bovensiepen Universität Duisburg-Essen Experimental Physics	Interface physics, surface science, non-linear optics, photoelectron spectroscopy, soft X-ray spectroscopy, ultrafast phenomena, solid-liquid interface
 Prof. Dr. Guido Clever Technische Universität Dortmund Bioinorganic Chemistry	Supramolecular coordination chemistry, self-assembled nanocages, chemistry in confined environments, photo-redox and stimuli-responsive systems
 Prof. Dr. Lukas J. Gooßen Ruhr-Universität Bochum Organic Chemistry I	Organometallic chemistry, photochemistry, electrochemistry, biofuels, homogeneous and heterogeneous catalysis, electronic data management, catalytic valorization of renewables
 Prof. Dr. Martina Havenith Ruhr-Universität Bochum Physical Chemistry II	Laser spectroscopy, linear and nonlinear terahertz (THz) spectroscopy, THz calorimetry, high-resolution infrared spectroscopy, microsolvation, ultracold chemistry
 Prof. Dr. Stefan Huber Ruhr-Universität Bochum Organic Chemistry II	Organocatalysis, noncovalent interactions, halogen/chalcogen bonding, supramolecular chemistry, organic synthesis, reaction kinetics, NMR/ITC titrations
 Prof. Dr. Stefan Kast Technische Universität Dortmund Theoretical Physical Chemistry	Liquid state theory, quantum-mechanical solvation models, reaction thermodynamics in solution, computational spectroscopy, hybrid solvation models for large systems

PERSON	RESEARCH FIELDS
 Prof. Dr. Rasmus Linser Technische Universität Dortmund Biomolecular NMR Spectroscopy	Solution and solid-state NMR spectroscopy, NMR techniques, integrated structural biology, protein structure and dynamics, protein-ligand interactions, protein-solvent interactions
 Prof. Dr. Benjamin List Max-Planck-Institut für Kohlenforschung Homogeneous Catalysis	Organocatalysis, asymmetric counteranion-directed catalysis (ACDC), amino catalysis, Brønsted acid catalysis, Lewis acid catalysis
 Prof. Dr. Dominik Marx Ruhr-Universität Bochum Theoretical Chemistry	Quantum simulations (ab initio, machine learning; path integral, bosonic, quasiclassical), theoretical liquid-state spectroscopy, nuclear quantum effects, proton transfer, cryochemistry
 Prof. Dr. Karina Morgenstern Ruhr-Universität Bochum Physical Chemistry I	STM techniques, chemistry in confined environments, isomerisation reactions, supported water structures, laser-induced surface reactions, kinetics of nanostructure formation
 Prof. Dr. Frank Neese Max-Planck-Institut für Kohlenforschung Molecular Theory and Spectroscopy	Method development in quantum chemistry, theoretical and experimental spectroscopy (X-Ray, EPR, MCD...), open shell species, reaction mechanisms, magnetism, ORCA program
 Prof. Dr. Jörg Neugebauer Max-Planck-Institut für Nachhaltige Materialien Computational Materials Design	Electronic structure methods, statistical physics, numerical algorithms, computational interface science, electrochemistry, corrosion, machine learning

PERSON	RESEARCH FIELDS
 Prof. Dr. Poul Petersen Ruhr-Universität Bochum Time-resolved Vibrational Spectroscopy	Linear and nonlinear infrared spectroscopy, surface-specific spectroscopy (SFG), 2D-IR spectroscopy, water structure and dynamics, proton transfer, hydrogen-bonded systems
 Prof. Dr. Gabriele Sadowski Technische Universität Dortmund Thermodynamics	Thermodynamic modelling of complex systems, thermodynamics, salt influence in biological systems, ion pairing, solvent influence on chemical and biological reactions
 Prof. Dr. Elsa Sánchez García Technische Universität Dortmund Computational Bioengineering	Computational regulation of enzymatic activity and protein engineering in solution, multiscale simulations, free energy calculations, molecular dynamics, data mining, machine learning
 Prof. Dr. Wolfram Sander Ruhr-Universität Bochum Physical Organic Chemistry	Physical organic chemistry, reactive intermediates, chemistry of open shell molecules, radicals, carbenes, synthesis and spectroscopy of peptides, matrix isolation spectroscopy, time resolved spectroscopy
 Prof. Dr. Lars Schäfer Ruhr-Universität Bochum Molecular Simulation	Theoretical biophysics, biomolecular simulation of protein condensation and aggregation, molecular engines, collective dynamics in solution, local thermodynamics in liquids
 Prof. Dr. Wolfgang Schuhmann Ruhr-Universität Bochum Analytical Chemistry	Analytical chemistry, (micro-) electrochemistry, scanning electrochemical microscopy (SECM), localized corrosion, fuel cell catalysts, biofuel cells, photoelectrochemistry

PERSON	RESEARCH FIELDS
 Prof. Dr. Kristina Tschulik Ruhr-Universität Bochum Analytical Chemistry II	Nano-electrochemistry, electrocatalysis, spectro-electrochemistry, electro-deposition, electrosynthesis, chemistry in confinement, charge transfer at interfaces
 Prof. Dr. Roland Winter Technische Universität Dortmund Biophysical Chemistry	X-ray & neutron scattering, calorimetry, CD, FT-IR, fluorescence spectroscopy & microscopy, AFM; high pressure biophysics; protein-lipid interactions; co-solvent & confinement effects on protein stability...

PARTICIPATING SCIENTISTS

PERSON	RESEARCH FIELDS
 Prof. Dr. Ulf-Peter Apfel Ruhr-Universität Bochum Electrosynthesis	Electrolysis and catalysis, scale-up and pilot plants of electrochemical processes, co- factor design for molecular energy conversion
 Prof. Dr. Jörg Behler Ruhr-Universität Bochum Theoretical Chemistry II	Theoretical chemistry, atomistic simulations, machine learning potentials, neural network potential energy surfaces, molecular dynamics, solid-liquid interfaces, liquid phase reactions
 Dr. Josep Cornella Max-Planck-Institut für Kohlenforschung Sustainable Catalysis for Organic Synthesis	Organic synthesis, transition metal and bismuth catalysis, development of synthetic methods and reagents, sustainable chemistry

PERSON	RESEARCH FIELDS
 Prof. Dr. Viktoria Däschlein-Gessner Ruhr-Universität Bochum Inorganic Chemistry II	Organometallic chemistry, reactive main group compounds, small molecule activation, homogeneous catalysis, ligand design, structure-activity relationships, machine learning
 Prof. Dr. Katrin F. Domke Universität Duisburg-Essen Electrochemical Surface Science	Electrochemical surface science, spectro-electrochemistry, near-field optics, Raman nanoscopy at electrified interfaces, redox-active molecules, electrocatalysis
 Prof. Dr. Ralf Drautz Ruhr-Universität Bochum Atomistic Modelling and Simulation	Atomistic modelling and simulation, electronic structure methods, machine learning and interatomic potentials, atomic cluster expansion (ACE) techniques
 Prof. Dr. Simon Ebbinghaus Ruhr-Universität Bochum Biophysical Chemistry	In-cell spectroscopy techniques, cosolutes and macromolecular crowding, protein folding and stability in cellulo, protein aggregation and liquid liquid phase separation, RNA stability
 Dr. André K. Eckhardt Ruhr-Universität Bochum Astrochemistry and Physical Organic Chemistry	Reactive intermediates, cryochemistry, matrix isolation spectroscopy, IR and EPR spectroscopy, astrochemistry, photochemistry, (in)organic synthesis
 Prof. Dr. Kai Exner Universität Duisburg-Essen Theoretical Inorganic Chemistry	Electrochemistry, electrocatalysis, theoretical electrochemistry, computational chemistry, multiscale modelling, descriptor-based approaches, electrocatalyst screening
 Prof. Dr. Hannsjörg Freund Technische Universität Dortmund Reaction Engineering and Catalysis	Reaction kinetics, hydrogenation reactions, selective oxidation, reactor design, multiphase reaction systems, heterogeneous catalysis, transport processes, process intensification

PERSON	RESEARCH FIELDS
 Prof. Dr. Christof Hättig Ruhr-Universität Bochum Quantum Chemistry	Electronic structure theory, coupled cluster response and embedding methods, computation of (non)linear spectra and reaction mechanisms in solution, TURBOMOLE program
 Prof. Dr. Richard Kramer Campen Universität Duisburg-Essen Chemical Physics of Interfaces	Heterogeneous chemistry at solid/liquid, air/liquid and gas/solid interfaces, femto(photo) electrochemistry, nonlinear optical spectroscopy, photo electrocatalysis
 Prof. Max M. Hansmann Technische Universität Dortmund Organic Chemistry	Organic synthesis, photo-/redox-functional and stimuli-responsive systems, organic radicals and polyradicals, reactive intermediates, strong nucleophiles, redox-systems
 Prof. Dr. Thomas Happe Ruhr-Universität Bochum Photobiotechnology	Biocatalysis, enzyme engineering, chemical biology, synthetic biochemistry, nanotechnology, nanomachines, biofuel cells, renewable energy
 Prof. Dr. Christian Herrmann Ruhr-Universität Bochum Physical and Biophysical Chemistry	Mutagenesis, bacterial recombinant protein synthesis and purification, site specific fluorescence labeling, transient kinetics, differential scanning calorimetry, isothermal titration calorimetry
 Prof. Dr. Müge Kasanmascheff Technische Universität Dortmund EPR Spectroscopy	Biocatalysis, advanced EPR spectroscopic techniques, structure-function relationship of proteins, metallocofactors, radical-carrying biomolecules, reactive intermediates

PERSON	RESEARCH FIELDS
 Dr. Elisabeth Kreidt Technische Universität Dortmund Lanthanoid Coordination Chemistry	Lanthanoid coordination chemistry, solvation effects on lanthanoid luminescence, paramagnetic NMR, circularly polarized luminescence, photoswitches
 Prof. Dr. Sebastian Kruss Ruhr-Universität Bochum Functional Nanomaterials	Fluorescence microscopy and spectroscopy (1D, 2D, near infrared, time resolved), functionalized carbon nanotubes, photophysics, biofunctionalization, biosensors
 Prof. Dr. Christian Merten Ruhr-Universität Bochum Stereochemistry and Chiroptical Spectroscopy	Chiroptical spectroscopy, vibrational circular dichroism, computational spectroscopy, cryospectroscopy, photochemical reactions of chiral molecules
 Dr. Celia Millon Ruhr-Universität Bochum Photonics and Ultrafast Laser Science	Laser technology and photonics toward industrial applications, start-up founder RayVen, ultrashort pulse, high-power laser
 Prof. Dr. Martin Muhler Ruhr-Universität Bochum Technical Chemistry	Heterogeneous catalysis, photocatalysis, electrocatalysis, catalyst synthesis, vibrational spectroscopy
 Prof. Dr. Edvardas Narevicius Technische Universität Dortmund Experimental and Theoretical Quantum Optics	Ultracold chemistry at mK conditions, experimental observation of quantum dynamics, development of novel molecular cooling methods
 Prof. Dr.-Ing. Marcus Petermann Ruhr-Universität Bochum Particle Technology	Supercritical fluids, unconventional solvents, antisolvent precipitation, electrochemical catalysis in supercritical fluids, sol-gel processes, thermo- and fluid dynamics at high pressures

PERSON		RESEARCH FIELDS
	Dr. Martin Rabe Max-Planck-Institut für Nachhaltige Materialien Interface Chemistry and Surface Technology	Interface spectroscopy, interface design and self assembly, eletrochemical interfaces, soft matter at interfaces, nanoscale IR spectroscopy
	Prof. Dr. Herre Jelger Risselada Technische Universität Dortmund Computational Interface Physics	Computational interface physics, coarse grain MD, artificial intelligence, optimization by artificial evolution, automated force-field optimization, recognition of fluid interfaces
	PD Dr. Michael Rohwerder Max-Planck-Institut für Nachhaltige Materialien Interface Chemistry and Surface Engineering	Molecular electrochemistry, local processes in the double layer, electrodes in the dry technique, in situ scanning Kelvin probe (SKP) force microscopy in synchrotron set-ups, corrosion protection
	Prof. Dr. Clara Saraceno Ruhr-Universität Bochum Photonics and Ultrafast Laser Science	Ultrafast, high power laser technology, THz sources, nonlinear optics, pulse shaping, spatiotemporal pulse propagation simulations
	Prof. Dr. Igor Schapiro Technische Universität Dortmund Theoretical Biophysics	Computational photochemistry, non-adiabatic MD, excited states, conical intersections, multiscale simulations, photoresponsive molecules, photocatalysis, multireference methods.
	Prof. Dr. Frank Schulz Ruhr-Universität Bochum Chemistry and Biochemistry of Natural Products	Enzymology, enzyme engineering, biocatalysis, biosynthesis, biotransformations, natural products, enzyme cascades, organic synthesis, bioactivity

PERSON	RESEARCH FIELDS
 Prof. Dr. Ferdi Schüth Max-Planck-Institut für Kohlenforschung Heterogeneous Catalysis	Heterogeneous catalysis, synthesis of materials with controlled porosity and nanostructured catalysts, energy relevant conversions, biomass conversion, ammonia decomposition, catalyzed hydrogen storage
 Prof. Dr. Katrin Sommer Ruhr-Universität Bochum Didactics of Chemistry	Didactics of chemistry, director of the Alfred Krupp-Schülerlabor RUB, Early Learners' Lab, public outreach, citizen science projects
 Prof. Dr. Marialore Sulpizi Ruhr-Universität Bochum Theoretical Physics of Electrified Solid/Liquid Interfaces	Ab initio molecular dynamics, electrified interfaces, computational electrochemistry, theoretical vibrational spectroscopy including Sum Frequency Generation, pKa calculations
 Prof. Dr. Jörg Tatzelt Ruhr-Universität Bochum Biochemistry of Neurodegenerative Diseases	Liquid-liquid phase separation, protein-protein interactions, protein-ligand interactions, protein-solvent interactions, protein folding and aggregation, solvent tuning
 PD Dr. Harun Tüysüz Max-Planck-Institut für Kohlenforschung Heterogeneous Catalysis and Sustainable Energy	Heterogeneous catalysis, sustainable energy, mesoporous materials, nanocasting, electrocatalysis, solar water splitting, oxygen evolution reaction, glycerol oxidation
 Dr. Ana Vila Verde Universität Duisburg-Essen Soft Matter and Interfaces	Atomistic simulations, polarizable and coarse grain force fields, solvation dynamics and thermodynamics, hydrophobic effect, biomolecule-solvent interactions

PERSON	RESEARCH FIELDS
 Prof. Dr. Siegfried R. Waldvogel Max-Planck-Institut für Chemische Energiekonversion Electrosynthesis	Electrosynthesis, electrifying industrial organic syntheses, organic electrochemistry, oxidative coupling reactions, synthesis of natural products and bioactive compounds
 Prof. Dr. Xijie Wang Technische Universität Dortmund /Universität Duisburg-Essen Ultrafast Electron Diffraction and Imaging	Liquid phase MeV ultrafast electron scattering and imaging in chemistry, free electron laser, high-brightness electron beam generation and applications
 Prof. Dr. Konstanze Winklhofer Ruhr-Universität Bochum Molecular Cell Biology	Advanced light microscopy, super-resolution structured-illumination microscopy, live cell imaging, liquid-liquid and liquid-solid phase transitions, protein aggregation