



















RESOLV 2012-2018: SCIENTISTS








PRINCIPAL INVESTIGATORS







AREA(S)	PERSON	RESEARCH FIELDS
A, C	 Prof. Dr. Christof Hättig Ruhr-Universität Bochum Theoretical Chemistry	Accurate electronic structure theory, coupled cluster response theory, weak / van der Waals / hydrogen-bonding interactions for large systems, external electromagnetic fields
A, B, C	 Prof. Dr. Martina Havenith Ruhr-Universität Bochum Physical Chemistry II	IR laser spectroscopy, molecular aggregates, THz absorption spectroscopy, solvation dynamics, laser development, Scattering Nearfield IR- and Raman- microscopy, ultracold chemistry
B	 Prof. Dr. Christian Herrmann Ruhr-Universität Bochum Physical Chemistry I	Protein thermodynamics in aqueous co-solvents and ionic liquids, enzymatic reactions, protein interactions, microcalorimetry, CD spectroscopy; kinetics, stopped flow, T-jump
A	 Prof. Dr. Benjamin List Max-Planck-Institut für Kohlenforschung Mülheim an der Ruhr	Development and mechanistic investigation of new methods of chemical synthesis, asymmetric organocatalysis and anion mediated asymmetric catalysis
A, B	 Prof. Dr. Dr. h.c. Wolfgang Lubitz Max-Planck-Institut für Chemische Energiekonversion Mülheim an der Ruhr	Paramagnetic Systems (radicals, triplet states, metal complexes), metalloproteins: wateroxidase, hydrogenase, ribonucleotide reductase; primary processes of photosynthesis; magnetic resonance spectroscopy; quantum chemical calculations
A, B, C	 Prof. Dr. Dominik Marx Ruhr-Universität Bochum Theoretical Chemistry	Ab initio (Car-Parrinello) molecular dynamics, theoretical spectroscopy, HPC, solvation, liquids, water, hydrogen-bonding, interfaces, charge transport, proton transfer, aggregation
A, C	 Prof. Dr. Karina Morgenstern Ruhr-Universität Bochum Physical Chemistry I	Surface science, surface reactions, non-adiabatic reactions, hydrogen bonding, kinetics of nanostructures, water, azobenzene derivatives, metallic surfaces, insulating layers, real space imaging, electron transfer excitation, femtosecond excitation







AREA(S)	PERSON	RESEARCH FIELDS
C	 <p>Prof. Dr. Martin Muhler Ruhr-Universität Bochum Technical Chemistry</p>	Heterogeneous catalysis, catalyst preparation, elucidation of elementary steps, redox catalysts in gas vs liquid phase, advanced spectroscopy coupled to transient kinetic methods
A, C	 <p>Prof. Dr.-Ing. Marcus Petermann Ruhr-Universität Bochum Particle Technology</p>	Product design from lab to industrial scale, separation techniques using supercritical fluids, thermo- and fluid dynamic data, sorption/desorption kinetics of gas mixtures at high pressure
A, B	 <p>Prof. Dr. Wolfram Sander Ruhr-Universität Bochum Organic Chemistry II</p>	Physical organic chemistry, reactive intermediates, chemistry of open shell molecules, radicals, carbenes, synthesis and spectroscopy of peptides, matrix isolation spectroscopy, time resolved spectroscopy
C	 <p>Prof. Dr. Ferdi Schüth Max-Planck-Institut für Kohlenforschung Mülheim an der Ruhr</p>	Fundamental studies of crystallization processes, catalysis, synthesis of catalyst materials, high throughput experimentation in catalysis, hydrogen storage materials, zeolites and ordered mesoporous materials, biomass transformation
A, C	 <p>Prof. Dr. Wolfgang Schuhmann Ruhr-Universität Bochum Analytical Chemistry</p>	Analytical chemistry, (micro-) electrochemistry, scanning electrochemical microscopy (SECM), localized corrosion, fuel cell catalysts, biofuel cells, photoelectrochemistry
C	 <p>Prof. Dr. Eckhard Spohr Universität Duisburg-Essen Theoretical Chemistry</p>	Classical and ab initio computer simulation of chemical reactivity and transport in electrolytes, near interfaces, in membranes, disordered media and in heterogeneous materials for energy research, development of reactive force fields for use in aqueous system simulations








AREA(S)	PERSON	RESEARCH FIELDS
C	 <p>Prof. Dr. Martin Stratmann Max-Planck-Institut für Eisenforschung GmbH Düsseldorf_</p>	Electrochemistry, corrosion science, buried interfaces, spectroscopy of electrified interfaces, surface science
B	 <p>Prof. Dr. Walter Thiel Max-Planck-Institut für Kohlenforschung Mülheim an der Ruhr</p>	Quantum chemistry and computational chemistry for large molecular systems, QM/MM techniques, spectroscopy, dynamics, reactivity, catalytic reactions and enzymatic processes
C	 <p>Prof. Dr. Metin Tolan Technische Universität Dortmund Experimental Physics I & DELTA</p>	Synchrotron radiation, interface scattering, small-angle X-ray scattering, X-ray spectroscopy, coherent X-ray scattering, soft condensed matter, biointerfaces, water networks
A, C	 <p>Prof. Dr.-Ing. Eckhard Weidner Ruhr-Universität Bochum Verfahrenstechnische Transportprozesse</p>	Supercritical fluids, phase equilibria/mass and heat transfer in multiphase systems, controlled release systems, micro- and nanoparticles, high pressure technology
B, C	 <p>Prof. Dr. Roland Winter Technische Universität Dortmund Physical Chemistry I</p>	X-ray and neutron scattering, calorimetry, CD, FT-IR, fluorescence spectroscopy, atomic force and fluorescence microscopy; structure, dynamics and function of model biomembranes, protein-lipid interactions; protein folding, misfolding and amyloidogenesis; co-solvent and confinement effects on protein stability and folding; high pressure effects in molecular biophysics









PARTICIPATING SCIENTISTS

AREA(S)	PERSON	RESEARCH FIELDS
B	 <p>Dr. Ulf-Peter Apfel Ruhr-Universität Bochum Inorganic Chemistry</p>	Activation and formation of biologically and industrially relevant small molecules
B	 <p>Prof. Dr. Enrica Bordignon Ruhr-Universität Bochum EPR Spectroscopy</p>	EPR spectroscopy, site-directed spin labeling, Double Electron-Electron Resonance, dynamic nuclear polarization, membrane protein structure-dynamics-function relationship, water dynamics, Bcl-2 proteins, apoptosis, ABC transporters, molecular biology
C	 <p>Prof. Dr. Uwe Bovensiepen Universität Essen-Duisburg Experimental Physics</p>	Electron and ion solvation dynamics at metal-molecule interfaces; Methods: Femtosecond time- and angle-resolved non-linear photoelectron spectroscopy
A	 <p>Prof. Dr. Guido Clever Technische Universität Dortmund Inorganic Chemistry II</p>	Supramolecular chemistry in solution, self-assembled coordination cages, confined molecular environments, host-guest chemistry, stimuli responsive systems, modified DNA nano structures; methods: NMR, CD spectroscopy, HRMS, isothermal titration calorimetry (ITC)
A	 <p>Prof. Dr. Viktoria Däschlein-Gessner Ruhr-Universität Bochum Inorganic Chemistry II</p>	Organometallic Chemistry: Tailoring structures and properties of carbanionic reagents for selective synthetic applications
A	 <p>Prof. Dr. Lukas J. Gooßen Ruhr-Universität Bochum Organic Chemistry I</p>	Development of catalytic methods, C-C, C-H and CO ₂ activation, fluoroalkylations, separations in supercritical fluids
B	 <p>Prof. Dr. Thomas Happe Ruhr-Universität Bochum Photobiotechnology</p>	Solvation effects on redox proteins; solvation shell dynamics on proton transfer within hydrogenases; Methods: Photocatalysis, enzyme technology, overexpression, purification and protein crystallography of anaerobic sensitive proteins

AREA(S)	PERSON	RESEARCH FIELDS
A	 <p>Prof. Dr. Stefan Huber Ruhr-Universität Bochum Organic Chemistry I</p>	Organocatalysis and supramolecular chemistry, multidentate halogen bonding in solution
B	 <p>Jun.-Prof. Dr. Müge Kasanmascheff Technische Universität Dortmund Physical Chemistry</p>	Electron paramagnetic resonance spectroscopy, hyperfine spectroscopy, amino acid radicals, metalloproteins, proton-coupled electron transfer reactions, ribonucleotide reductases, unnatural amino acid incorporation
A, B	 <p>Prof. Dr. Stefan Kast Technische Universität Dortmund Theoretical Physical Chemistry</p>	Liquid state theory in combination with molecular dynamics and quantum chemistry; solvation effects on structure, spectra and thermodynamics in chemical and biological systems
B	 <p>Prof. Dr. Rasmus Linser Technische Universität Dortmund Physical Chemistry II</p>	Development of NMR spectroscopic methods (proton detection in solid-state NMR, fast Magic-Angle Spinning), protein dynamics, protein-ligand and protein solvent interactions using NMR spectroscopy
A	 <p>Dr. Christian Merten Ruhr-Universität Bochum Organic Chemistry II</p>	Intermolecular interactions and chiral induction studied by vibrational CD
B	<p>Prof. Dr. Nils Metzler-Nolte Ruhr-Universität Bochum Bioinorganic Chemistry I</p>	Synthesis of bioconjugates of metal complexes with peptides and peptide nucleic acid oligomers. Tailor-made peptides of increasing complexity, in particular polypeptide/metal complexes
B	 <p>Prof. Dr. Franz Narberhaus Ruhr-Universität Bochum Microbial Biology</p>	Synthesis of temperature-labile & "RNA thermometers"; and characterization of their unusual properties in terms of hydration effects; Methods: small to medium RNA synthesis, rational design of point mutations, enzymatic and chemical probing of RNA structures, RNA-RNA and RNA-protein interactions, bioinformatic prediction of RNA structures

AREA(S)	PERSON	RESEARCH FIELDS
A	 <p>Prof. Dr. Frank Neese Max-Planck-Institut für Chemische Energiekonversion, Mülheim an der Ruhr</p>	Theoretical Method Development, ab initio wavefunctions, experimental and theoretical spectroscopy (X-Ray, EPR, MCD, absorption, resonance Raman), open shell transition metals, reaction mechanisms, magnetism, ORCA, bioinorganic chemistry
C	 <p>Prof. Dr. Jörg Neugebauer Max-Planck-Institut für Eisenforschung GmbH Düsseldorf</p>	Computational Materials Design
A	 <p>Prof. Dr. Patrick Nürnberger Ruhr-Universität Bochum Physical Chemistry II</p>	Time-resolved spectroscopy, ultrafast photochemistry, transient absorption, quantum control of photochemical reactions, real-time observation of excited-state processes, transfer phenomena, solvation effects, reaction intermediates
A, B	 <p>Prof. Dr. Poul Petersen Ruhr-Universität Bochum Time-resolved Vibrational Spectroscopy</p>	Development of nonlinear vibrational spectroscopic methods (ultrafast continuum IR and 2D IR spectroscopy, heterodyned SFG spectroscopy, chiral SFG spectroscopy, interferometric 2D SFG spectroscopy); vibrational spectroscopy of water in solvation shells, at surfaces, and in biological settings, strongly hydrogen-bonded complexes, proton transfer reactions, and surface-bound molecular catalysts
B	 <p>Prof. Dr. Nicolas Plumeré Ruhr-Universität Bochum Molecular Nanostructures</p>	Design and synthesis of solvated matrices for integration of redox-active molecules toward applications in catalysis, energy conversion and sensing
A	 <p>Prof. Dr.-Ing. Markus Richter Ruhr-Universität Bochum Thermodynamics</p>	Accurate thermophysical property measurements and investigation of the phase behavior (gas-to-liquid) taking account of surface phenomena (adsorption, capillary condensation, bulk condensation)

AREA(S)	PERSON	RESEARCH FIELDS
B	 <p>Prof. Dr. Matthias Rögner Ruhr-Universität Bochum Biochemistry of Plants</p>	<p>Solvent channels in control of catalytic center solvation in water-splitting Photosystem 2; Methods: Photoelectrochemistry, quantitative mass spectrometry, SPR, purification of intrinsic membrane protein complexes, fluorescence- & CD-spectroscopy</p>
C	 <p>Dr. Michael Rohwerder Max-Planck-Institut für Eisenforschung GmbH Düsseldorf</p>	<p>Kelvin probe, electrochemistry in the “dry”, structure of electrochemical double layer</p>
B	 <p>Dr. Michael Römelt Ruhr-Universität Bochum Theoretical Chemistry</p>	<p>Molecular simulation of molecules with complex electronic structures, Density Matrix Renormalization Group</p>
C	 <p>Prof. Dr. Axel Rosenhahn Ruhr-Universität Bochum Analytical Chemistry</p>	<p>Biointerfaces, biofouling, advanced surface chemistry, in-situ interface analysis, X-ray imaging, microfluidic adhesion experiments, 3D tracking</p>
A	 <p>Prof. Dr. Gabriele Sadowski Technische Universität Dortmund Biochemical and Chemical Engineering</p>	<p>Thermodynamic modeling of complex systems, biothermodynamics, salt influence in biological systems, ion pairing, solvent influence on chemical and biological reactions</p>
A, B	 <p>Prof. Dr. Elsa Sanchez Garcia University Duisburg-Essen, Computational Biochemistry</p>	<p>Multiscale methods, Quantum Mechanics and Molecular Dynamics simulations, free energy calculations. Biomolecules, catalysis and reactive intermediates</p>
B	 <p>Prof. Dr. Clara Saraceno Ruhr-Universität Bochum Photonics and Ultrafast Laser Science</p>	<p>High-power ultrafast solid-state lasers, nonlinear optics, high-power terahertz sources</p>

AREA(S)	PERSON	RESEARCH FIELDS
B	 <p>Prof. Dr. Lars Schäfer Ruhr-Universität Bochum Theoretical Chemistry</p>	Molecular simulation, biological macromolecules, molecular dynamics, force fields, multiscale modeling
C	 <p>Prof. Dr. Rochus Schmid Ruhr-Universität Bochum CMC</p>	Charge transfer at electrolyte/electrode interfaces; Methods: Coupling of periodic real-space DFT code to the Poisson-Boltzmann approach
B	 <p>Prof. Dr. Frank Schulz Ruhr-Universität Bochum Organic Chemistry I</p>	Bioorganic chemistry, natural products chemistry, enzymology
-	 <p>Prof. Dr. Katrin Sommer Ruhr-Universität Bochum Didaktik der Chemie</p>	Didactics and chemical education, model experiments
C	 <p>Prof. Dr. Kristina Tschulik Ruhr-Universität Bochum Lehrstuhl für Analytische Chemie II</p>	Nano-Electrocatalysis, Magneto-Electrochemistry, Electrodeposition
B	 <p>Prof. Dr. Jörg Tatzelt Ruhr-Universität Bochum Biochemistry of Neurodegenerative Diseases</p>	Prion and prion-like mechanisms, neurodegeneration, intrinsically disordered proteins, subcellular targeting, transport across membranes
A	 <p>Priv.-Doz. Harun Tüysüz Max-Planck-Institut für Kohlenforschung Mülheim an der Ruhr</p>	Design and development of nanostructured multifunctional materials for catalytic applications
B	 <p>Prof. Dr. Konstanze Winklhofer Ruhr-Universität Bochum Molecular Cell Biology</p>	Protein misfolding and aggregation, proteostasis, ubiquitination, life cell imaging, structured illumination (SIM) super-resolution imaging