Institute of Physical and Theoretical Chemistry

Prof. Dr. Sigurd Bauerecker

Researcher's Career

- Full Professor for Physical Chemistry, TU Braunschweig
- Heisenberg Professor, TU Braunschweig
- Research Periods at the ETH Zurich
- Group Leader, Helmholtz-Zentrum Geesthacht
- Dr. rer. nat. at the TU Braunschweig
- Study of Physics, Chemistry, Electrical Engineering, Braunschweig

Funding

DFG, DAAD, Helmholtz, VolkswagenStiftung, Industry

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Mission Statement

Our investigation of gas-phase molecules, aerosol particles and droplets is motivated by multiple factors such as: a better basic understanding of matter between molecule and bulk; their prominent role in the physics and chemistry of the atmospheres of the Earth, other planets, satellites and in space; their impact on weather and climate; the prospects of molecular aerosols and nanoparticles in health care, pharmacy and technical applications.

Research

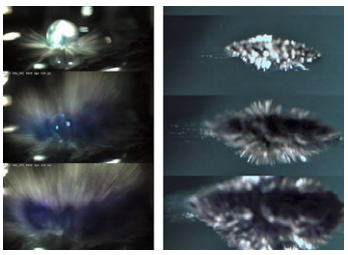
Objects of interest are supercooled gas molecules, molecular clusters (0.1 – 3 nm), molecular nanoparticles (3 – 1000 nm) and microparticles in the aerosol phase (1 – 10 µm), as well as acoustically levitated droplets (0.3 – 6 mm).

Particle properties are investigated as size and size distribution; shape (spherical, cubic, elongated, oblate, prolate, needleshaped, dendritic, …); state of aggregation (liquid, solid); phase (crystalline I, crystalline II, metastable, …); structure (crystalline, amorphous, core-shell, nanocomposite, covered surface, quasi-liquid layer, …); vibrational and scattering spectra, optical constants; intermolecular interactions (hydrogen and van der Waals bonding).

Particle and aerosol dynamics are in the focus of our research regarding size evolution (particle growth, decay, Ostwald ripening); shape evolution (spherical to elongated, dendritic growth), special phase transitions (freezing, melting, sublimation, desublimation, change between crystalline phases); molecular diffusion in nanoparticles; particle agglomeration.

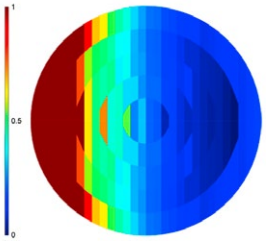
Experimental particle generation is performed by the following techniques: gas aggregation via optical long-path collisional cooling cells with adjustable temperature (4 – 400 K) and pressure (< 0.01 – 3000 mbar); sample-gas inlet techniques such as pulse-injection, (enclosive) flow cooling∞ acoustic trapping and levitation; climate chambers; laser heating, evaporation and desorption. The collisional cooling cells have been constructed, patented and upgraded together with industrial partners. Twin systems of these cells are used in a few collaborations.

Particle and aerosol characterization is realized by FTIR spectroscopy (rapid-scan, low- and high-resolution) in the 400 – 10000 cm^{-1} range; visible (VIS) and infrared (IR) high-speed imaging (analyses of fast processes such as freezing of supercooled droplets); and supported by methods of computational chemistry (ab initio, molecular dynamics, Monte Carlo, Mie calculations, discrete dipole approximation) together with collaboration partners.



Coulombic explosion of a sodium droplet in water with "blue" solvated electrons.

Dendritc freezing of a supercooled water droplet.



Portion of dendritic ice after stage-one freezing.

Publications and Patents

- T. Buttersack, S. Bauerecker: Critical radius of supercooled water droplets: on the transition toward dendritic freezing, J. Phys. Chem. B, 120 (2016) 504-512, http://pubs.acs.org/doi/abs/10.1021/acs.jpc
- O.N. Ulenikov, E.S. Bekhtereva, Yu.V. Krivchikova, V.A. Zamotaeva, T. Buttersack, C. Sydow and S. Bauerecker: Study of the high resolution spectrum of 32S16O18O: the ν1 and ν3 bands, (2015) J. Quant. Spectrosc. Radiat. Transfer, 168 (2016) 29-39, http://dx.doi.org/10.1016/j.jqsrt.2015.08.010.
- P.E. Mason, F. Uhlig, V. Vaněk, T. Buttersack, S. Bauerecker, and P. Jungwirth: Coulomb explosion at early stages of the reaction of alkali metals with water, Nature Chemistry 7 (2015) 250-254.
- S. Bauerecker, T. Buttersack: Electric effect during the dendritic freezing of supercooled water droplets, J. Phys. Chem. B, 118 47 (2014) 13629-13635, http://pubs.acs.org/doi/abs/10.1021/jp507440a.
- A.V. Nikitin, V. Boudon, Ch. Wenger, S. Albert, L.R. Brown, S. Bauerecker and M. Quack: High resolution spectroscopy and the first global analysis of the Tetradecad region of methane 12CH4, Phys. Chem. Chem. Phys. 15 (2013) 10071-10093, DOI: 10.1039/c3cp50799h.