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Roman M Balabin

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Spectroscopy and Mass-spectrometry in Physical and Analytical Chemistry of Biological Systems and Industrial Products

Roman M. Balabin, PhD

BWAN – BrainWare Analytics, Zurich, Switzerland

BSH – Bond Street Holdings, Charlestown, Nevis

Outline

Part I. Bio / CV

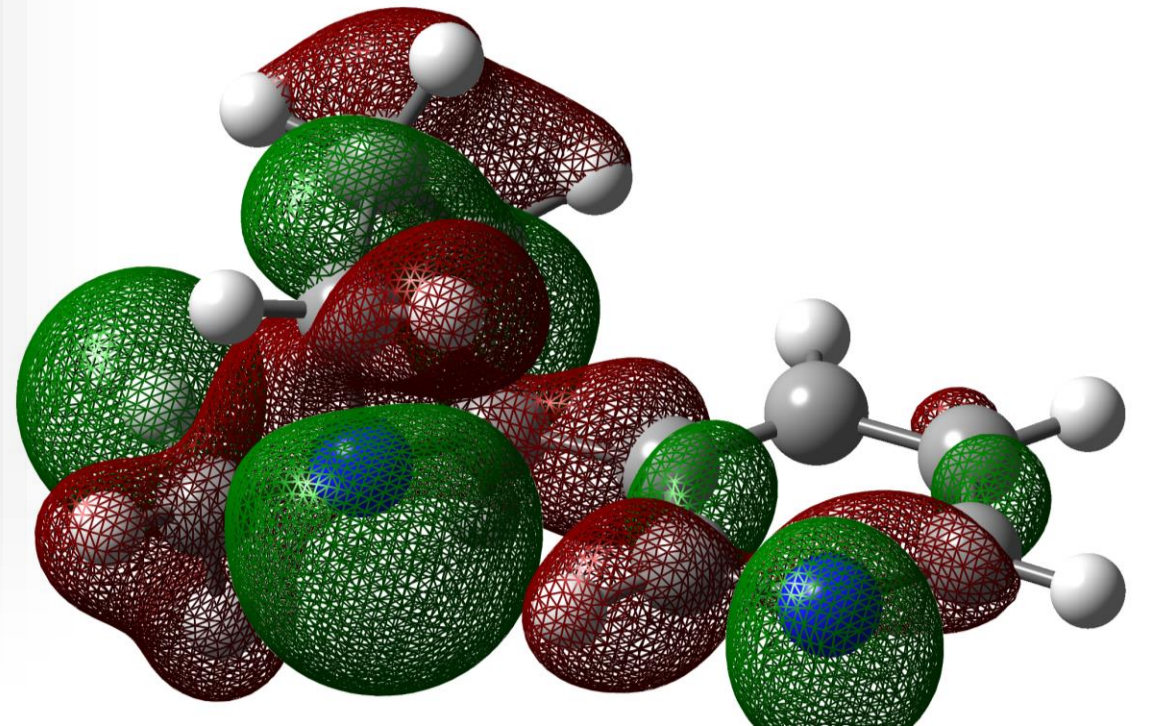
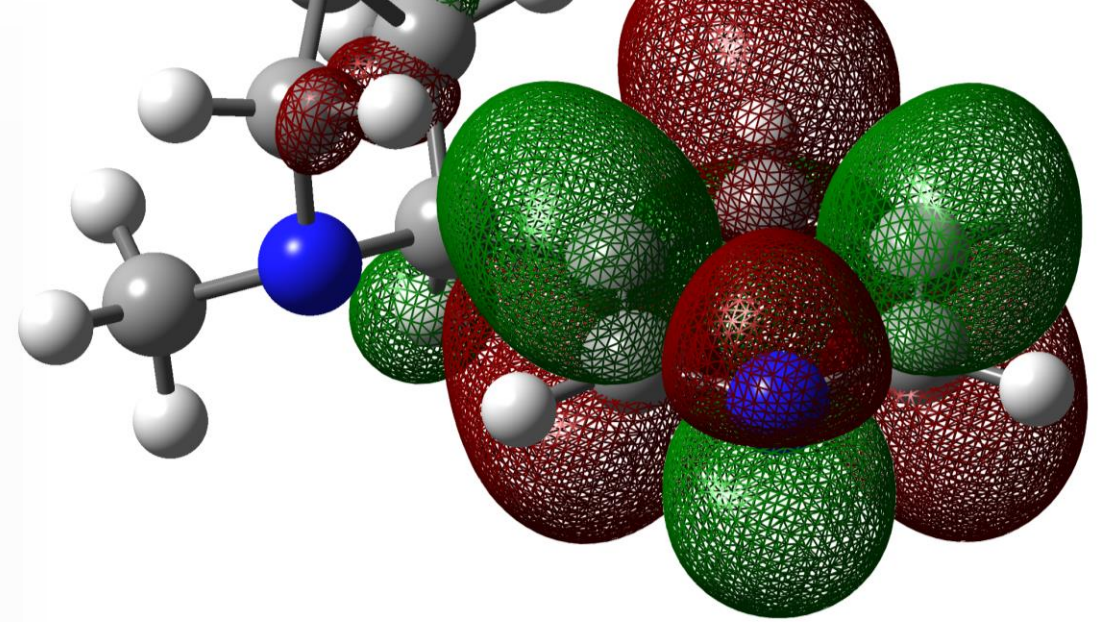
Part II. Results:
Petroleum macromolecules and
surface science

Part II. BrainWare Analytics GmbH

Part III. The HyDRA Challenge

Part IV. Triplets (de)activation

Part V. Above the ground(state)



Part I. Bio / CV

Early Years: 1985–2002

- Name: **Roman M. Balabin** (*Роман Балабин*)
 - ORCID: [0000-0001-9374-1809](https://orcid.org/0000-0001-9374-1809)
 - ResearcherID: [M-7662-2019](https://pubs.academia.edu/M-7662-2019)
 - Scopus ID: [15049329900](https://scopus.com/authorid/15049329900)
- Born on August 21, 1985, in the Cheryomushki (Brezhnevsky) district of **Moscow**, USSR
- Family:
 - Mother: Irina V. Balabina (Ivanova; 1960, Moscow)
 - Father: Mikhail I. Balabin (Shegidevich; 1961, Moscow)
 - Grandfather: Izmail Yakovlevich Shegidevich (Izmail Jakubowicz Szegidewicz) – repressed nobleman of Polish-Tatar origin



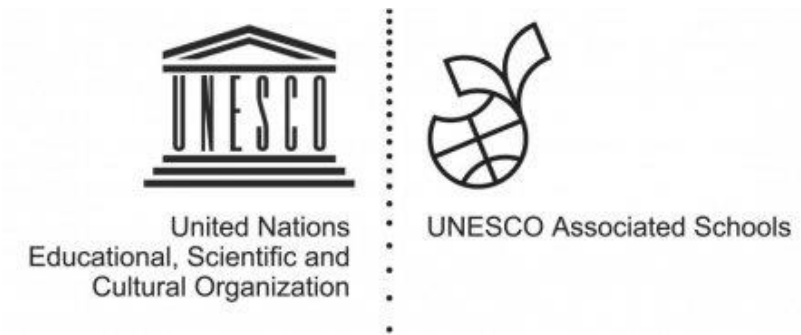
Early Years: 1985–2002

- Lived on Khersonskaya and Volgina str. (Moscow)
- Summer vacations in **Spassk** (Bednodemyanovsk) of Penza Oblast, especially in 1992–1994
- Shortly lived in **Anapa** (Kuban, 1988–1989), **Pyatigorsk** (Stavropolye, 1990), **Sochi** (1991) and **Tallin** (1990–1991)
- First travel to Western Europe, **Rome**, in Aug 1995
- Moved to **Blaibach** (Oberpfalz, Bayern, Germany) in 1996–1997
- Lived in **Zandt** (Oberpfalz, Bayern) in 1998



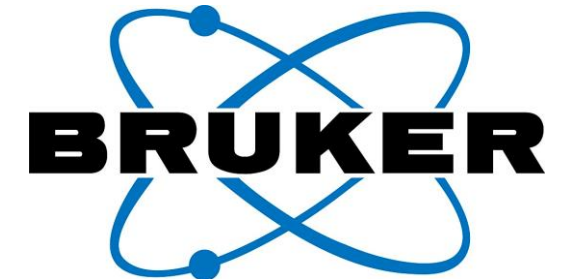
School Education

- Primary school No. 1655 / No. 15 (Khersonskaya, Moscow)
- School No. 562 / No. 15 (Perekopskaya, Moscow)
- School No. 1073 (Varshavskoe, Moscow) with its program authored by **Vladimir Myskin**
- Information Technology Lyceum No. 1533 “LIT” (Lomonosovsky) from 2000 to 2002 – **UNESCO** Associated Schools Project Network (ASPnet)
 - Computer science, math and IT
 - Diploma thesis with **Aleksandr Giglavyj**: “Information and communication technology (ICT) market of the Baltic states” (2002)



University Years: 2002–2008

- Uni: **Gubkin University** of Oil and Gas (Moscow)
 - Faculty of Chemical Engineering and Ecology
 - Department of Organic Chemistry and Petrochemistry
 - Major: chemistry and technology of **natural gas**
- Scientific collaborations:
 - **Bruker Optics** (Bremen, Germany)
 - ITERA / ARETI Group (Geneva, Switzerland)
 - Department of Physics, **Umea University** (Sweden)
 - Institute of Problems of Chemical Physics (Chernogolovka, Moscow Oblast)
 - Nesmeyanov Institute of Organoelement Compounds



University Years: 2002–2008

- Uni: **Gubkin University** of Oil and Gas (Moscow)
 - Faculty of Chemical Engineering and Ecology
 - Department of Organic Chemistry and Petrochemistry
 - Major: chemistry and technology of **natural gas**
- Industrial partners:
 - **Lumex** Instruments (St. Petersburg)
 - Orsknefteorgsintez / RussNeft (Orenburg Oblast)
 - Kirishinefteorgsintez / Kinef (Leningrad Oblast)
 - Astrakhan Gas Processing Plant / Gazprom
 - Kuibyshevsky Refinery (Samara Oblast)
 - The Ryazan Refinery / TNK-BP (Ryazan Oblast)



Pre-doc Studies: 2007–2008

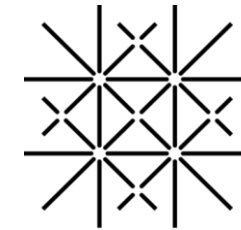
- Georg August University of **Göttingen** (Germany)
 - Institute of Physical Chemistry
 - Graduate school: Spectroscopy of molecular aggregates (GRK 782 PCGG, GEPRIS 273443)
 - Group of Prof. Dr. **Martin Suhm** / Philipp Zielke
 - Topic: Raman spectroscopy of normal alkanes
- Ruprecht Karl University of **Heidelberg** (Germany)
 - Institute of Applied Physical Chemistry
 - Group of Prof. Dr. **Michael Grunze** / Patrick Koelsch
 - Topic: sum-frequency-generation spectroscopy (SFGS) of biofilms



Pre-doc Studies: 2007–2008

- University of **Basel** (Switzerland)
 - Department of Chemistry
 - Group of Prof. Dr. **John Paul Maier** / Egor Chasovskikh
 - Topic: electronic spectroscopy of carbon radicals and ions (SNSF 115864)
 - Theoretical calculations: Université Paris-Est, Laboratoire de Chimie Théorique (France)

- Max Planck Institute for Polymer Research in **Mainz**
 - Experimental Physics of Interfaces @ MPI-P
 - Group of Prof. Dr. **Hans-Jurgen Butt** / Gunter Auernhammer
 - Invited talk on physical chemistry and spectroscopy of petroleum macromolecules



Universität
Basel

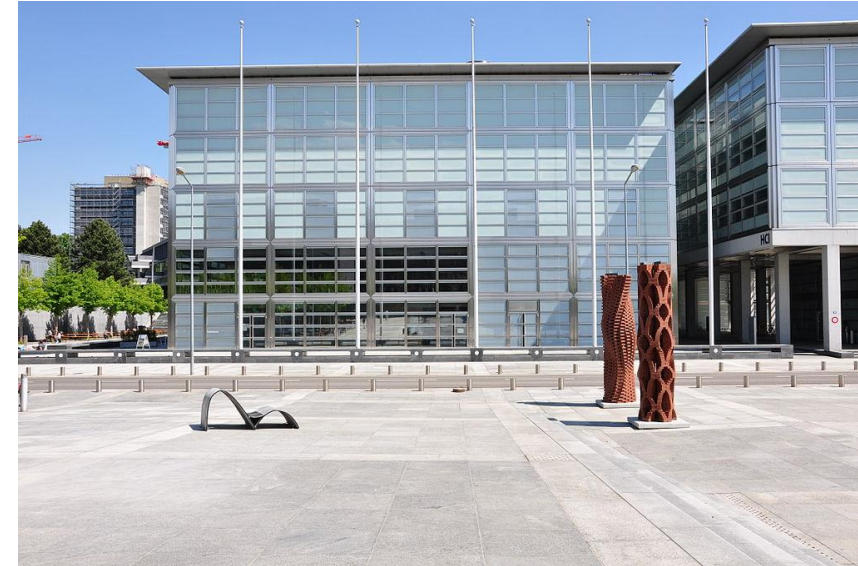
Max-Planck-Institut
für Polymerforschung

Max Planck Institute
for Polymer Research



PhD Studies: 2008–2012

- Uni: **ETH Zurich** (Switzerland)
 - Department of Chemistry and Applied Biosciences (D-CHAB)
 - Group of Prof. Dr. **Renato Zenobi**
 - Vibrational spectroscopy and mass-spectrometry
 - PhD thesis: “Development of express methods for analysis of petroleum refining products and petrochemicals based on vibrational spectroscopy” (Gubkin University, 2013)
- Industrial partners:
 - **Danone** Research Centre Daniel Carasso (Paris)
 - Unimilk (Moscow Oblast)
 - NT-MDT (Zelenograd, Moscow)



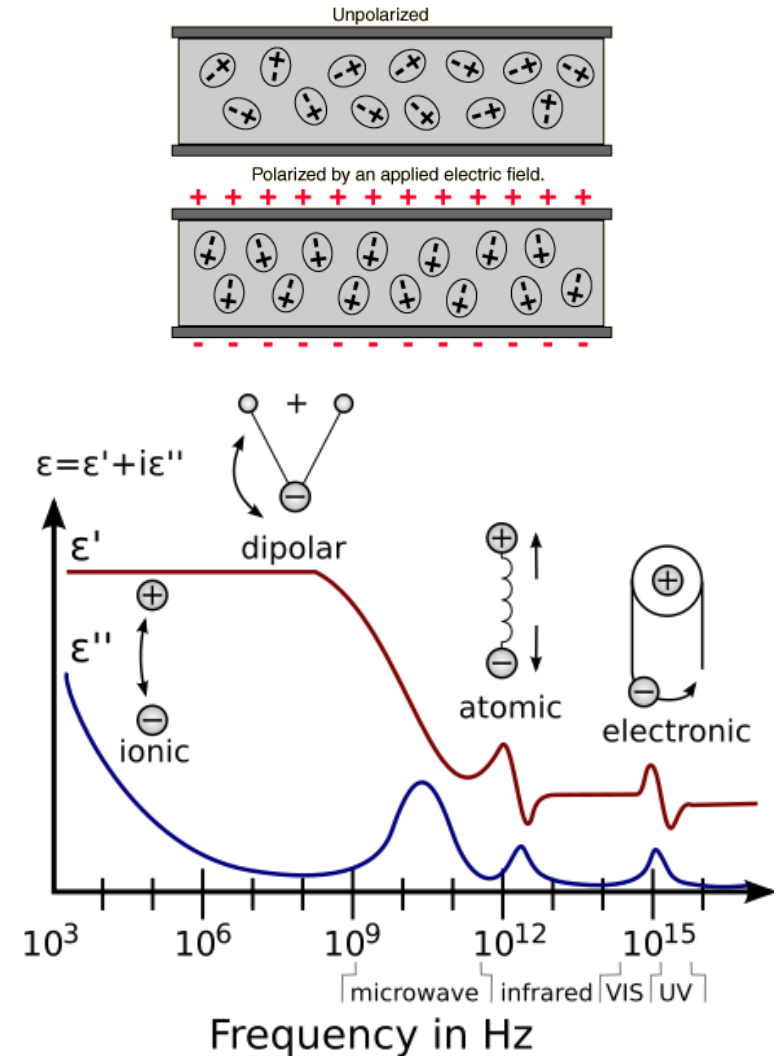
Part II. Results

Petroleum macromolecules and surface science



Dielectric spectroscopy: permittivity

- **Dielectric spectroscopy of oil:**
 - Paper “Frequency Dependence of Oil Conductivity at High Pressure” (2007)
 - Method: Dielectric spectroscopy (DS, impedance spectroscopy)
 - DS measures the dielectric properties of a medium as a function of applied frequency.
 - DS is based on the interaction of an external field with the electric **dipole moment** of the sample.
 - The result is expressed by **complex permittivity**.





Dielectric spectroscopy: model

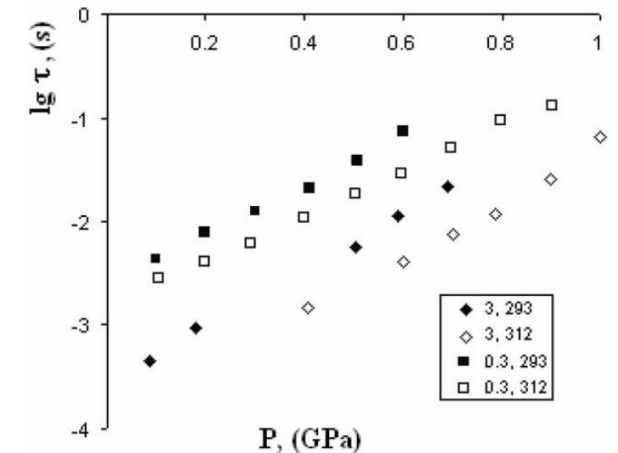
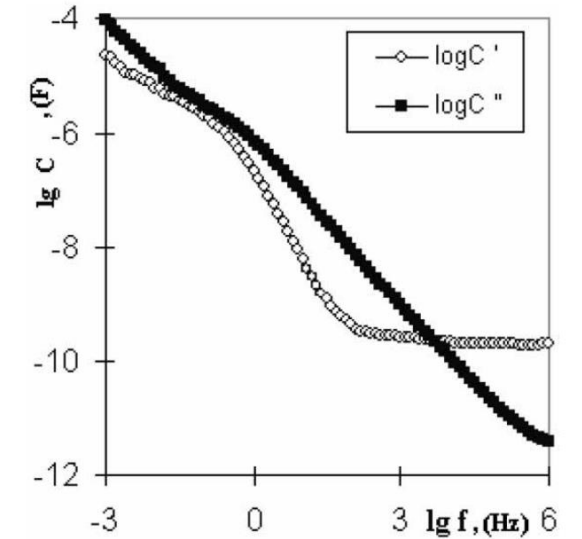
- **Dielectric spectroscopy of oil:**

- Paper “Frequency Dependence of Oil Conductivity at High Pressure” (2007)
- Samples:
 - Toluene solutions of asphaltene
 - Concentration of 0.3% (2.7 g/L) and 3% mass. (27 g/L)
- Conditions:
 - Temperatures of 312 and 294 K
 - Pressure: 0.1–1.0 GPa

- **Model:**

$$\frac{\epsilon^* - \epsilon_\infty}{A(i\omega)^n - \epsilon_\infty} = (1 + i\omega\tau)^{-1}$$

- Alternative to Jonscher’s “universal dielectric response” (UDR, 1977).



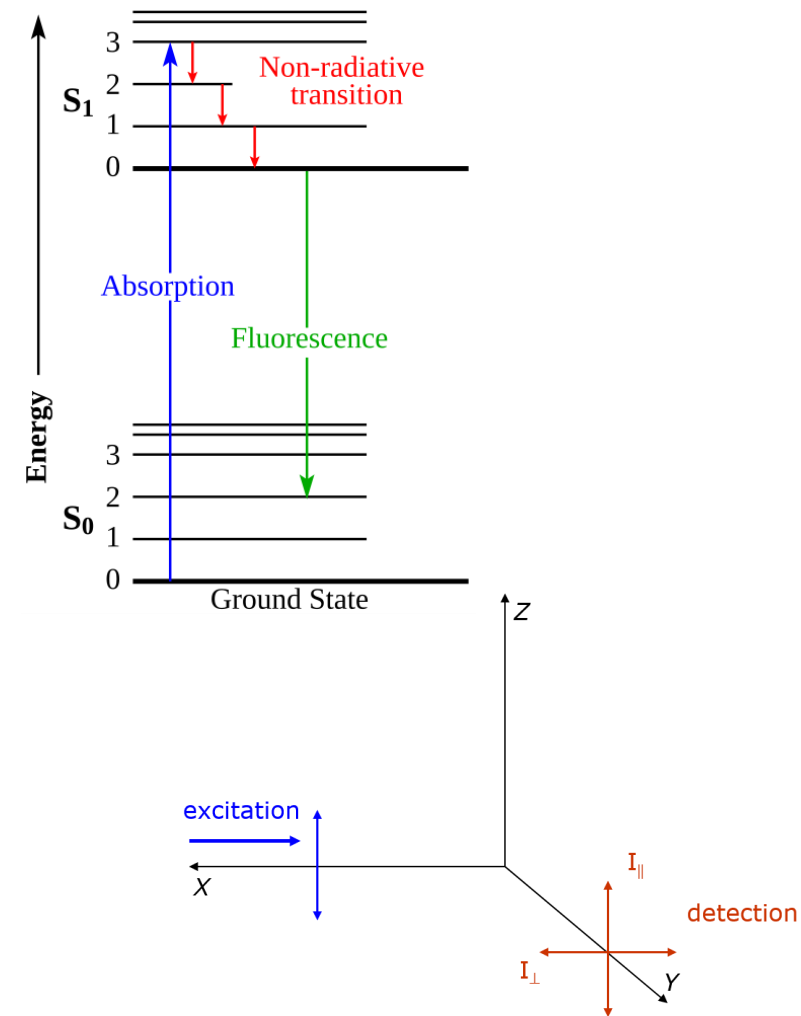


Fluorescence anisotropy

- **Fluorescence polarization** of asphaltenes:

- Paper “Polarization of Fluorescence of Asphaltene Containing Systems” (2008)
- Method: **Fluorescence spectroscopy** (fluorimetry or spectrofluorometry)
 - A complementary technique is absorption spectroscopy.
- Oil fluorophores are asphaltenes as they contain several combined aromatic groups.
- Anisotropy by Levshin for **monodispersed** systems:

$$\left(1 - \frac{3}{2} \sin^2 \xi\right) \left(\frac{1}{P} - \frac{1}{3}\right) = \frac{1}{P_0} - \frac{1}{3}$$





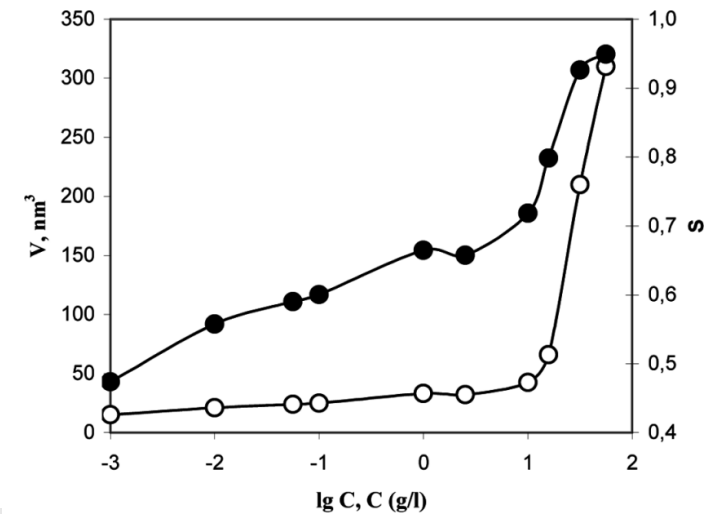
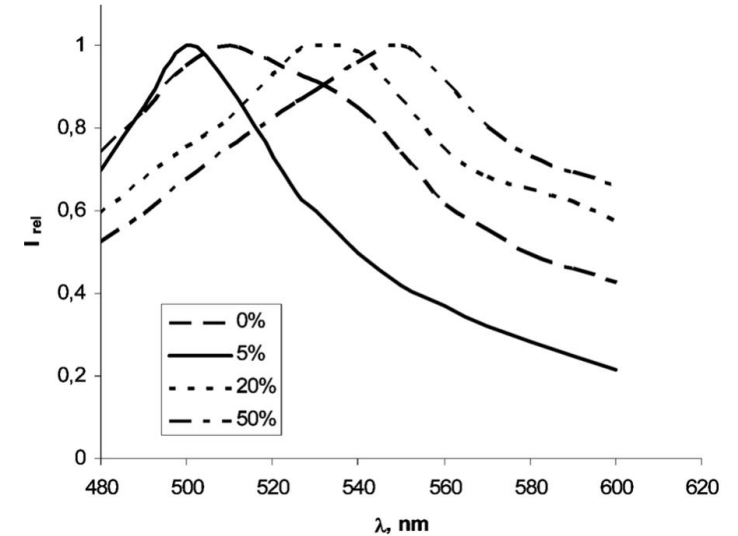
Fluorescence anisotropy

- **Fluorescence polarization** of asphaltenes:

- Paper “Polarization of Fluorescence of Asphaltene Containing Systems” (2008)
- Sample:
 - Asphaltenes in CCl_4 or toluene
 - Light catalytic gasoil, LCG
 - Distillate cracking residue, RCD

- Anisotropy for **polydisperse** (nonuniform) systems:

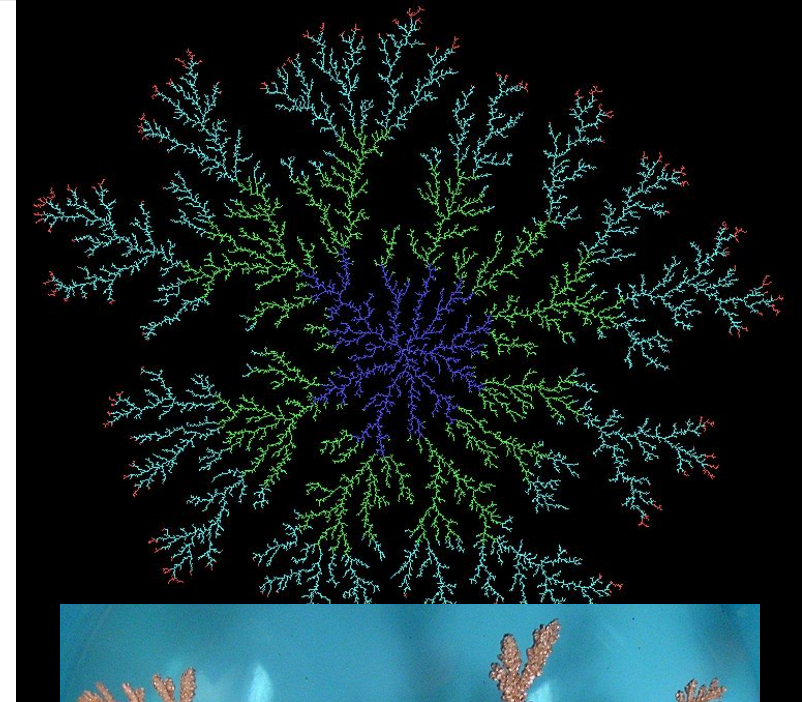
$$\frac{1}{P} = \frac{1}{3} + \left(\frac{1}{P_0} - \frac{1}{3} \right) \frac{\int \omega_V(V) dV}{\int \frac{V \omega_V(v) dV}{\frac{\tau k T}{\eta} + V}} = \frac{1}{3} + \left(\frac{1}{P_0} - \frac{1}{3} \right) \frac{1}{S}$$





Dipole Moment of Fractal Cluster

- **Molecular dynamics** of asphaltenes:
 - Paper “Calculation of Dipole Moment of Fractal Asphaltene Cluster” (2011)
 - Method: **diffusion-limited aggregation (DLA)**
 - a random walk due to Brownian motion and a cluster process to form fractal aggregates
 - Diffusion is the primary means of transport.
 - Mansoori and colleagues have created a model based on the concept of fractal structure of asphaltene clusters.





Dipole Moment of Fractal Cluster

- **Molecular dynamics** of asphaltenes:

- Paper “Calculation of Dipole Moment of Fractal Asphaltene Cluster” (2011)

- System:

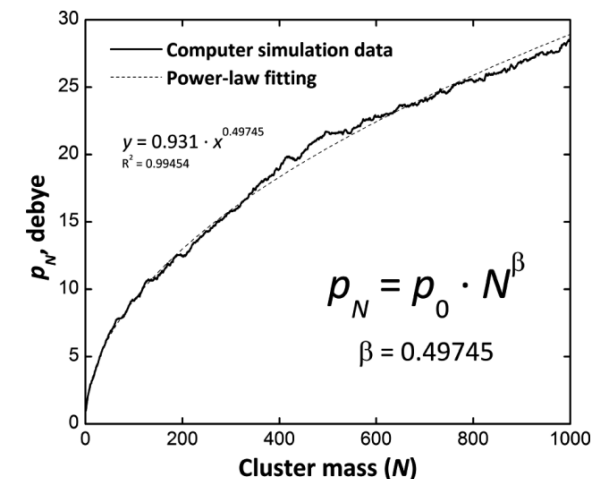
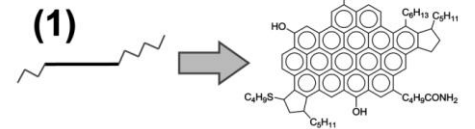
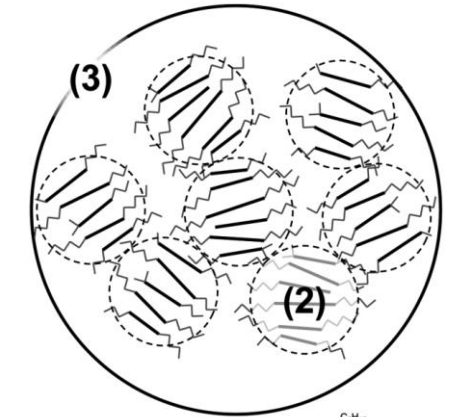
- petroleum pitch – as it possesses paramagnetic properties

- The dipole moment of the asphaltene cluster was demonstrated to vary according to **power law** in relation to the cluster mass.

- The dipole-dipole interactions between the asphaltene nanoaggregates increase.

- Analytical solution:

$$p_N = p_0 \cdot N^\beta; \quad \beta = \frac{4}{15} \cdot \frac{p_0^2}{4\pi\epsilon_0\epsilon k_B T r^3}$$

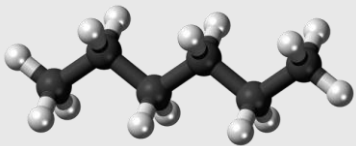


Other Results



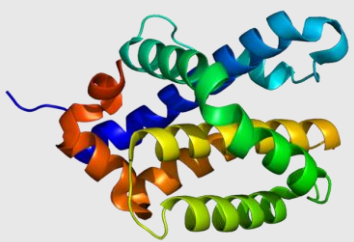
Scientific and industrial results

- Machine learning for **vibrational spectroscopy** data:
 - A series of papers on near-infrared spectroscopy of petrochemicals, products of petroleum refining and biofuels:
 - [Fuel \(2007\) 323](#), [Energy Fuels \(2007\) 2460](#), [Chemom Intell Lab Syst \(2007\) 183](#), [Fuel \(2008\) 1096](#), [Chemom Intell Lab Syst \(2008\) 58](#), [Fuel \(2008\) 2745](#), [Neural Comput Appl \(2009\) 557](#), [ACA \(2010\) 27](#), [Analyst \(2011\) 1703](#), [ACA \(2011\) 190](#), [ACA \(2011\) 63](#), [Fuel \(2011\) 2007](#), [Microchem J \(2011\) 121](#), [Energy Fuels \(2011\) 2373](#), [Analyst \(2012\) 1604](#).
 - Practical implementation for laboratory analysis at Kinef (Kirishi), Samara, **Gazprom** (Astrakhan) and Mozyr Refinery (Belarus)
- **Petroleum macromolecules** and surface science:
 - A series of papers on asphaltenes, petroleum resins and other colloid systems:
 - [JDST \(2007\) 419](#), [JNIRS \(2007\) 343](#), [JDST \(2008\) 457](#), [JCIS \(2008\) 167](#), [JDST \(2008\) 1505](#), [Energy Fuels \(2009\) 1230](#), [Energy Fuels \(2011\) 189](#), [JDST \(2011\) 1502](#), [Phys Wave Phen \(2015\) 143](#).
 - Colloid state control of **Kumkol oil** (Kazakhstan)



Scientific and industrial results

- Physical chemistry of **normal alkanes**:
 - A series of papers on quantum chemistry and Raman spectroscopy of alkanes:
 - [Chem Phys \(2008\) 267](#), [JCP \(2008\) 164101](#), [JPCA \(2009\) 1012](#), [JPCA \(2010\) 6729](#), [Mol Phys \(2011\) 943](#).
 - The **benchmark** experimental value for the enthalpy difference between *trans* and *gauche* conformations of normal butane: $\Delta H = 660 \pm 22 \text{ cal mol}^{-1}$
 - Used by Bachrach in [Computational Organic Chemistry](#) (2014), Vogel & Houk in *Organic Chemistry* (2019), AMBER FF for biomolecules, etc.
- **Machine learning** for quantum chemistry:
 - One of the **earliest** attempts to combine ML and QC:
 - [JCP \(2009\) 074104](#), [PCCP \(2011\) 11710](#).
 - Almost zero interest after publication, but became a large separate field of studies in 2020s: ML-DFT, ML-FF, Δ -learning, etc.
 - Review by Dral in [Quantum Chemistry in the Age of Machine Learning](#) (2022) 698 pp.



Scientific and industrial results

- Physical chemistry of **biomolecules**:
 - A series of papers on QC and Raman spectroscopy of gas-phase **amino acids**:
 - [Chem Phys Lett \(2009\) 195](#), [PCCP \(2010\) 5980](#), [JPCL \(2010\) 20](#), [JCP \(2010\) 231101](#), [JPCB \(2010\) 15075](#), [Comput Theor Chem \(2011\) 15](#), [PCCP \(2012\) 99](#).
 - The very first measurement of **conformation equilibrium in free glycine**
 - QC of other biomolecules – triazoles, tetrazole, formic acid, aldehydes, etc.:
 - [JCP \(2009\) 154307](#), [JPCA \(2009\) 4910](#), [JPCA \(2010\) 3698](#), [JCP \(2010\) 211103](#), [JASMS \(2011\) 1167](#), [Struct Chem \(2011\) 1047](#), [Mol Phys \(2011\) 2341](#), [PCCP \(2023\) 22089](#).
- **Mass-spectrometry** and electronic spectroscopy:
 - Food samples, dyes, peptides, biocomplexes, etc.:
 - [Analyst \(2010\) 773](#), [PCCP \(2010\) 11710](#), [PCCP \(2010\) 14121](#), [JASMS \(2010\) 172](#), [Angewandte \(2010\) 2358](#), [Anal Chem \(2010\) 7394](#), [ABC \(2010\) 405](#), [IJMS \(2011\) 241](#), [RSCA \(2011\) 1962](#).
 - Proof that electrospray ionization (ESI) generates **gaseous analytes at ambient conditions**

Journalist

- **Business-Swiss**, Zurich
 - Edited by Marad Widmer, LL.M.
 - Shveytsariya Delovaya / Widmer Strategy GmbH
- **Nasha Gazeta**, Geneva
 - Edited by Dr. Nadia Sikorsky (Nadezhda Sikorskaya)
 - Interview with *brigadier* Fredy Keller (SWISSINT)
- **Wikinews**, Miami, FL
 - Interviews with Profs. Jonathan Gruber (MIT), Clive Spash (CSIRO), Stephen Ward (UBC), Robert Costanza (UCL)

Швейцария Деловая



Part II. BrainWare Analytics GmbH

BrainWare Analytics: formal

- Formal: **Brainware Analytics GmbH** (Switzerland)
 - BrainWare Analytics LLC (BWAN)
 - EU VAT: CHE-202.748.777
 - Commercial register CH-170.4.011.342-9
 - Statutory date: 10 Jul 2012
 - Daily register No. 9743 / Publication number: 6791860
 - Official address: Rathausstrasse 14, 6340 Baar, Zug
 - Industry: computer hardware, provision of IT services
 - Share capital: 20'000 CHF
 - Registered persons: “Balabin, Roman, Russian citizen, in Schlieren, managing director, with sole signature and shareholder” (SHAB)



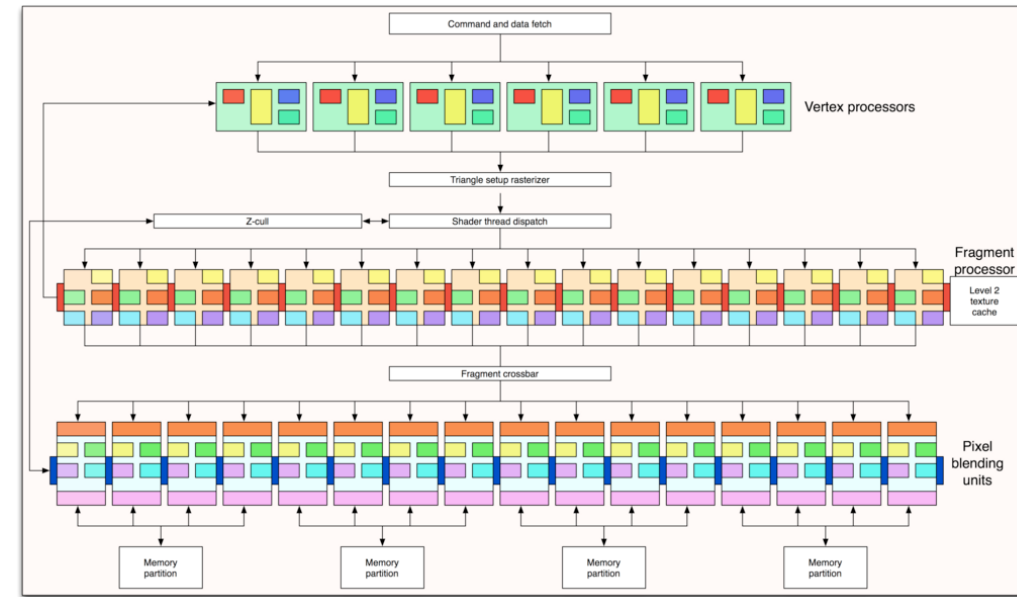
BrainWare Analytics: locations

- Office in **Schlieren**, 2013–2014:
 - Address: Grabenstrasse 11a, 8952 Schlieren, Zurich
 - Partner: Dualsystems Biotech AG
 - proteomics for industry and academia
- Office at **Technopark Zurich**, 2014–2017:
 - Address: Newton 1.OG, Technopark Zurich, Technoparkstrasse 1, 8005 Industriequartier, Zurich
 - Five people in Jul 2014:
 - two scientists with PhDs, two computer engineers and an expert in GPU-based computer simulations
 - “Balabin, Roman, Russian citizen, in Schlieren, managing director, with sole signature and shareholder... Kornilov, Pavel, Russian citizen, in Zurich, shareholder, without signatory power” (SHAB)



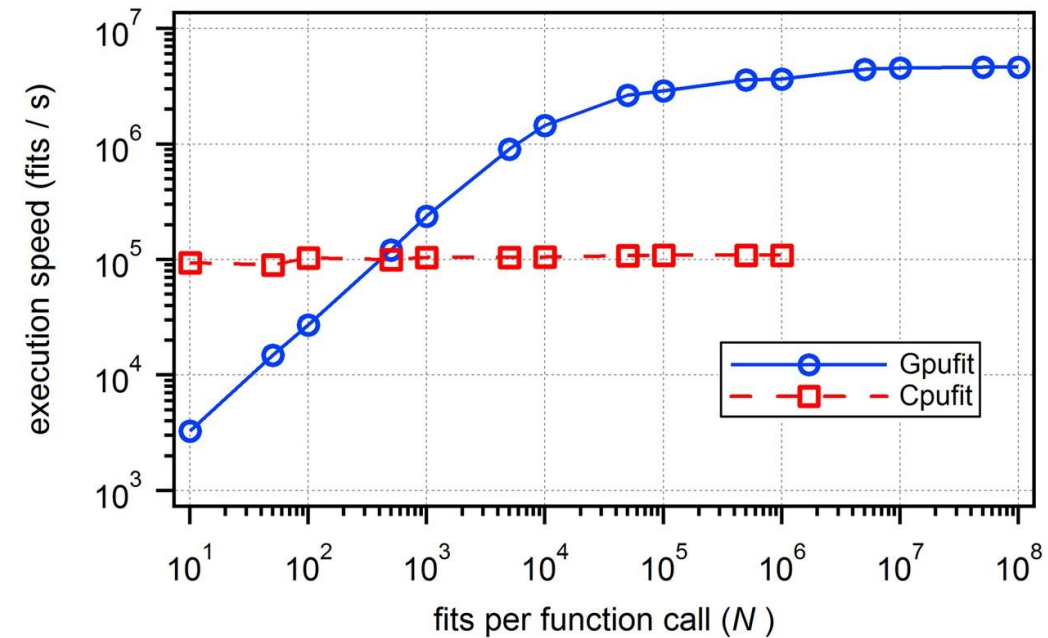
General-purpose computing on GPUs

- **GPGPU** = the use of a graphics processing units (GPUs) beyond computation of computer graphics only
- GPUs could perform computation in applications traditionally handled by the central processing unit (CPU)
- Fits **scientific computing**
- The use of multiple video cards in one computer further parallelizes the processing



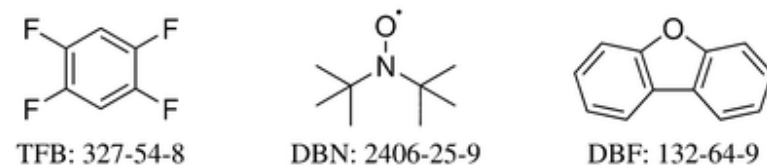
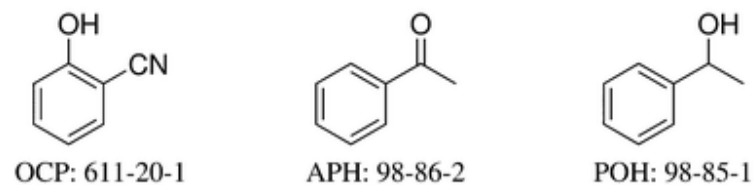
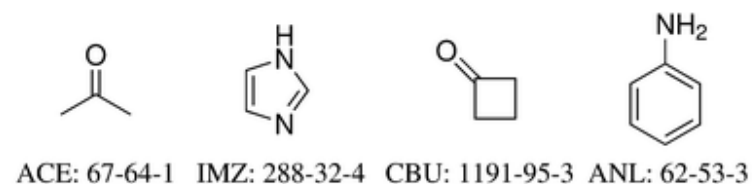
General-purpose computing on GPUs

- **GPGPU** = the use of a graphics processing units (GPUs) beyond computation of computer graphics only
- GPUs could perform computation in applications traditionally handled by the central processing unit (CPU)
- Fits **scientific computing**
- Example: estimation of non-linear parameters by the **Levenberg-Marquardt algorithm**



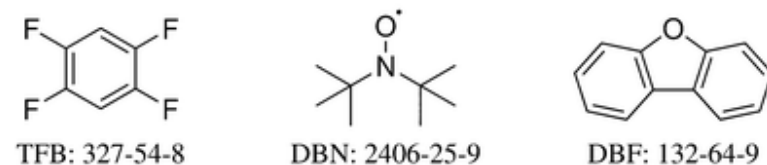
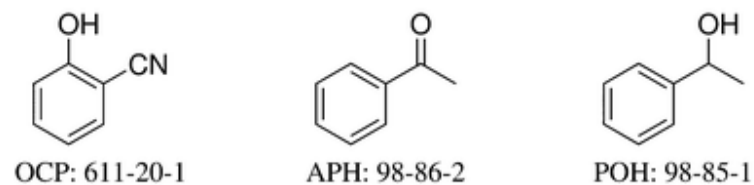
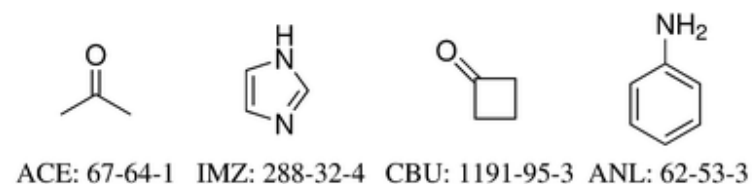
Part III. The HyDRA Challenge

The HyDRA Challenge



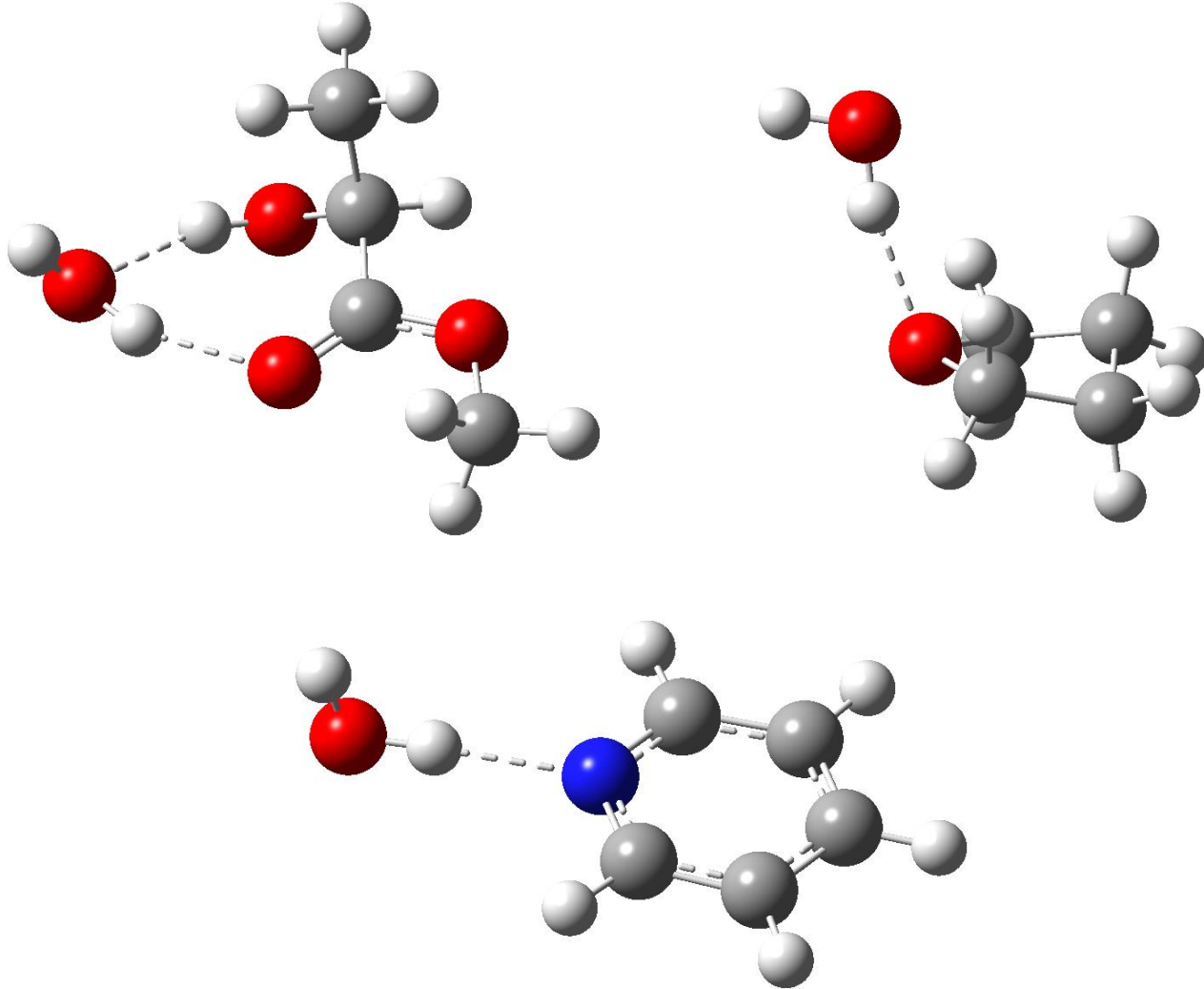
- **Hydrate Donor Redshift Anticipation (HyDRA)** blind challenge for the microhydration
- Organizers:
 - University of Göttingen / Paris-Saclay University
 - Prof. Dr. **Ricardo Mata** (theor) / Prof. Dr. **Anne Zehnacker-Rentien** (exp)
- Ten complexes of organic molecules with water
- No experimental information prior to predictions' submission (before Mar 2022)

The HyDRA Challenge



- The role of theory in understanding hydration is multifaceted:
 - Helps to **assign** the experimental spectral data
 - Could even **replace** experiment (to some extent)
- A need for **unbiased** tests of different predictive theoretical approaches by experiment

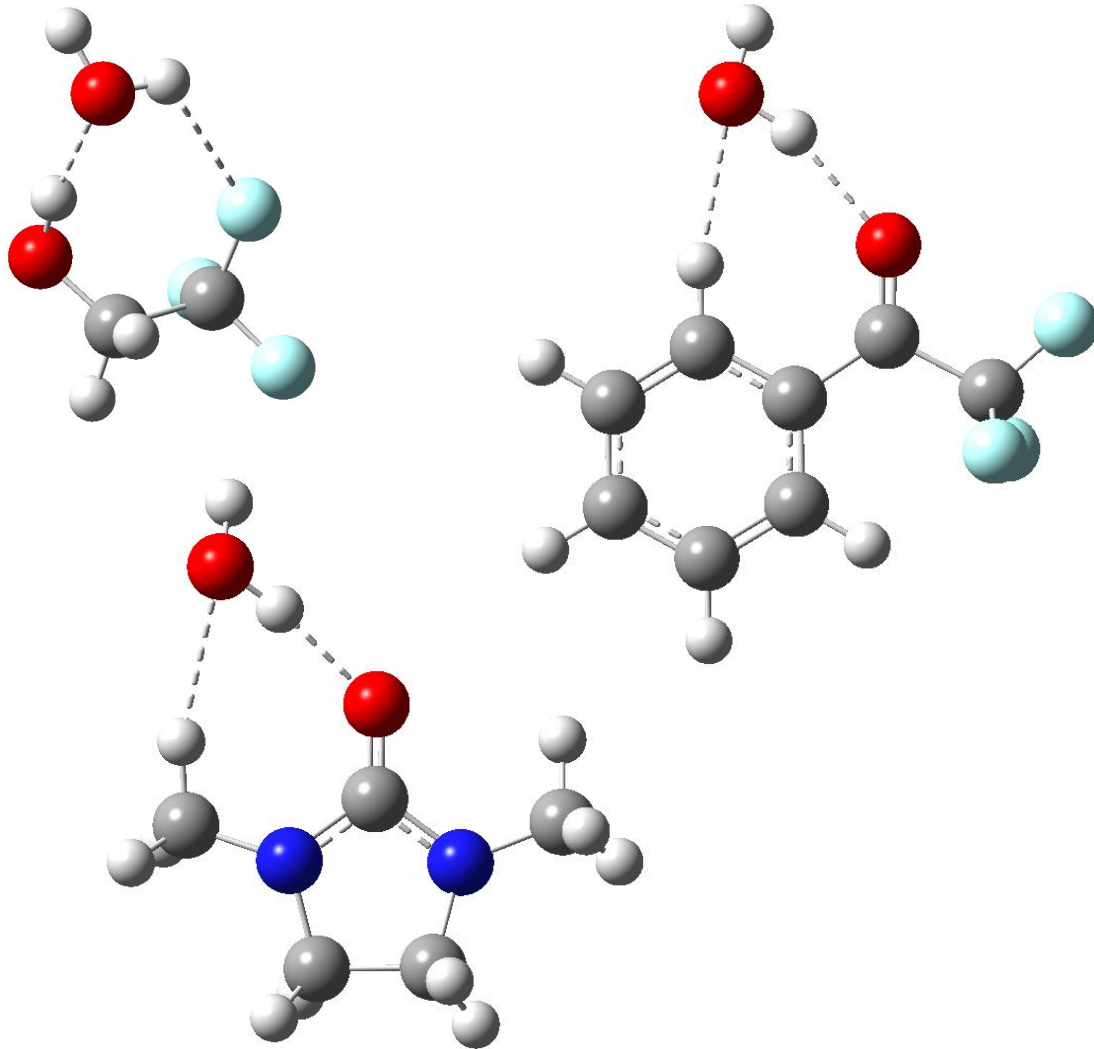
The HyDRA Challenge: structures



- The role of theory in understanding hydration is multifaceted:
 - Helps to **assign** the experimental spectral data
 - Could even **replace** experiment (to some extent)

- A need for **unbiased** tests of different predictive theoretical approaches by experiment

The HyDRA Challenge: structures



- To predict the **hydrogen-bonded** OH bond stretching fundamental of water in clusters
- Relative to the free water value of app. 3657 cm^{-1}
- Experimental **symmetric stretch**
- Starting date of Phase I: Feb 2021
- The official start: 24 Aug 2021

Part IV. Triplets (de)activation

Singlet states vs Triplet states

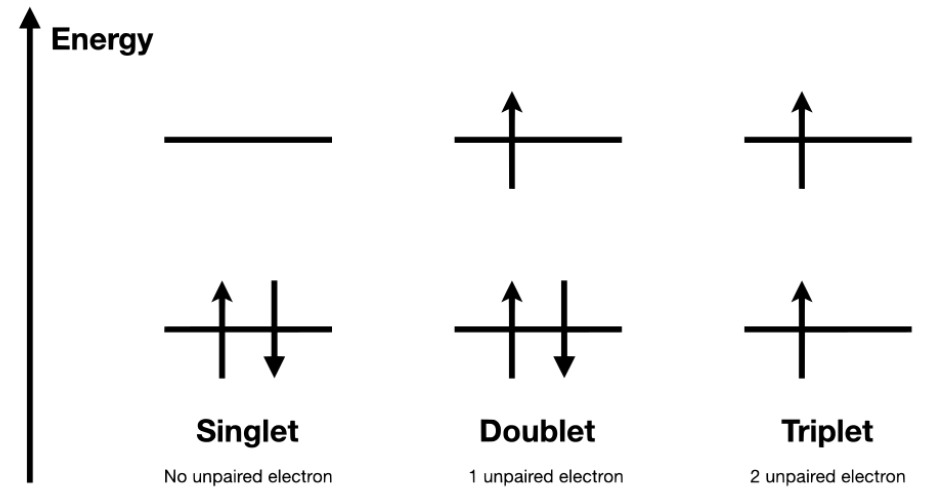
- **Clebsch–Gordan coefficients:**

$$\left| \frac{1}{2}, +\frac{1}{2} \right\rangle \otimes \left| \frac{1}{2}, +\frac{1}{2} \right\rangle \text{ by } (\uparrow\uparrow),$$

$$\left| \frac{1}{2}, +\frac{1}{2} \right\rangle \otimes \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \text{ by } (\uparrow\downarrow),$$

$$\left| \frac{1}{2}, -\frac{1}{2} \right\rangle \otimes \left| \frac{1}{2}, +\frac{1}{2} \right\rangle \text{ by } (\downarrow\uparrow),$$

$$\left| \frac{1}{2}, -\frac{1}{2} \right\rangle \otimes \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \text{ by } (\downarrow\downarrow)$$



- There are three states with total spin angular momentum of one

Singlet states vs Triplet states

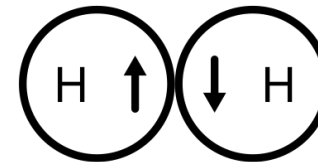
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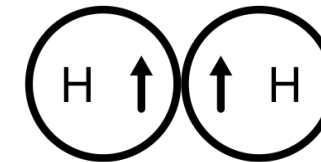
$$\left| \frac{1}{2}, +\frac{1}{2} \right\rangle \otimes \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \text{ by } (\uparrow\downarrow),$$

$$\left| \frac{1}{2}, -\frac{1}{2} \right\rangle \otimes \left| \frac{1}{2}, +\frac{1}{2} \right\rangle \text{ by } (\downarrow\uparrow),$$

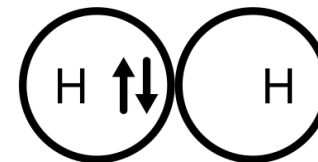
$$\left| \frac{1}{2}, -\frac{1}{2} \right\rangle \otimes \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \text{ by } (\downarrow\downarrow)$$



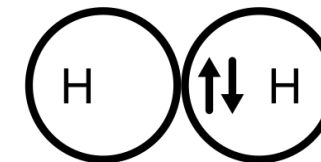
Heiter-London



Triplet



Ionic Form 1



Ionic Form 2

- There are three states with total spin angular momentum of one

Photon Upconversion

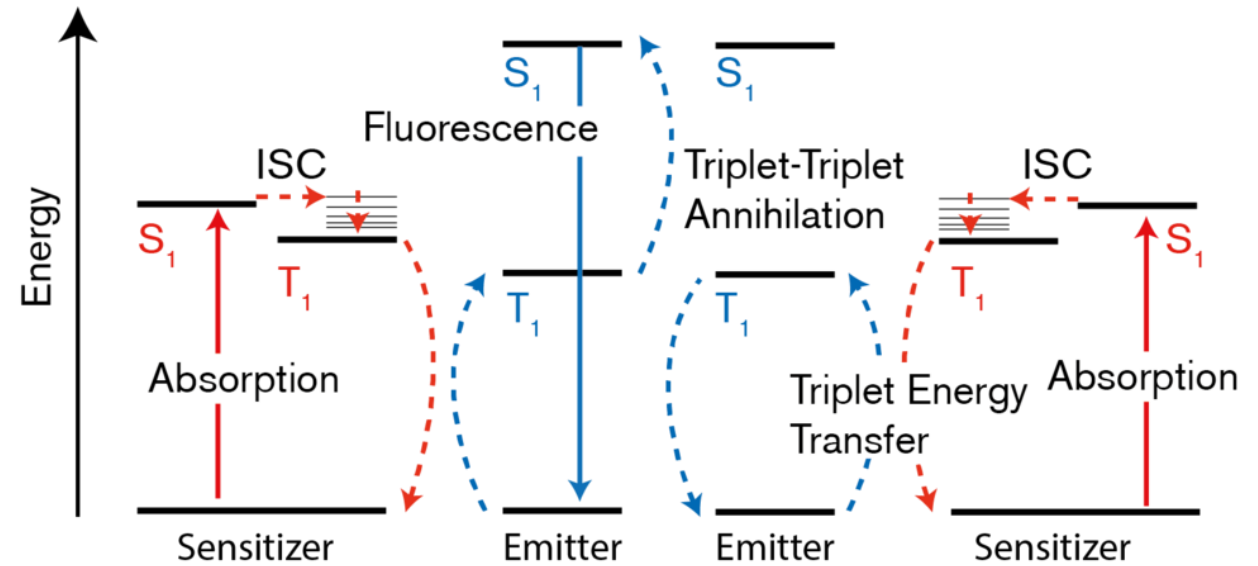
- **Clebsch–Gordan coefficients:**

$$\left| \frac{1}{2}, +\frac{1}{2} \right\rangle \otimes \left| \frac{1}{2}, +\frac{1}{2} \right\rangle \text{ by } (\uparrow\uparrow),$$

$$\left| \frac{1}{2}, +\frac{1}{2} \right\rangle \otimes \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \text{ by } (\uparrow\downarrow),$$

$$\left| \frac{1}{2}, -\frac{1}{2} \right\rangle \otimes \left| \frac{1}{2}, +\frac{1}{2} \right\rangle \text{ by } (\downarrow\uparrow),$$

$$\left| \frac{1}{2}, -\frac{1}{2} \right\rangle \otimes \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \text{ by } (\downarrow\downarrow)$$



- Triplet-triplet annihilation / **Dexter** electron transfer

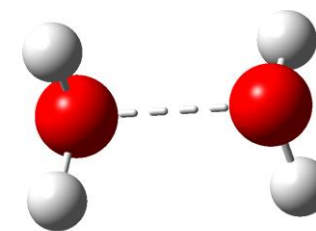
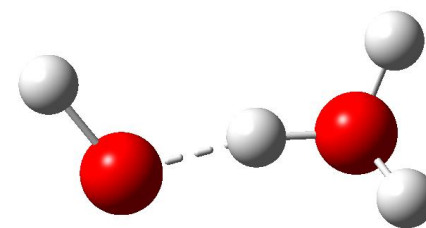
WDRAC: Water dimer radical-cation

The WDRACs, $(\text{H}_2\text{O})_2^{+\bullet}$, react with organic substances in three rather different ways:

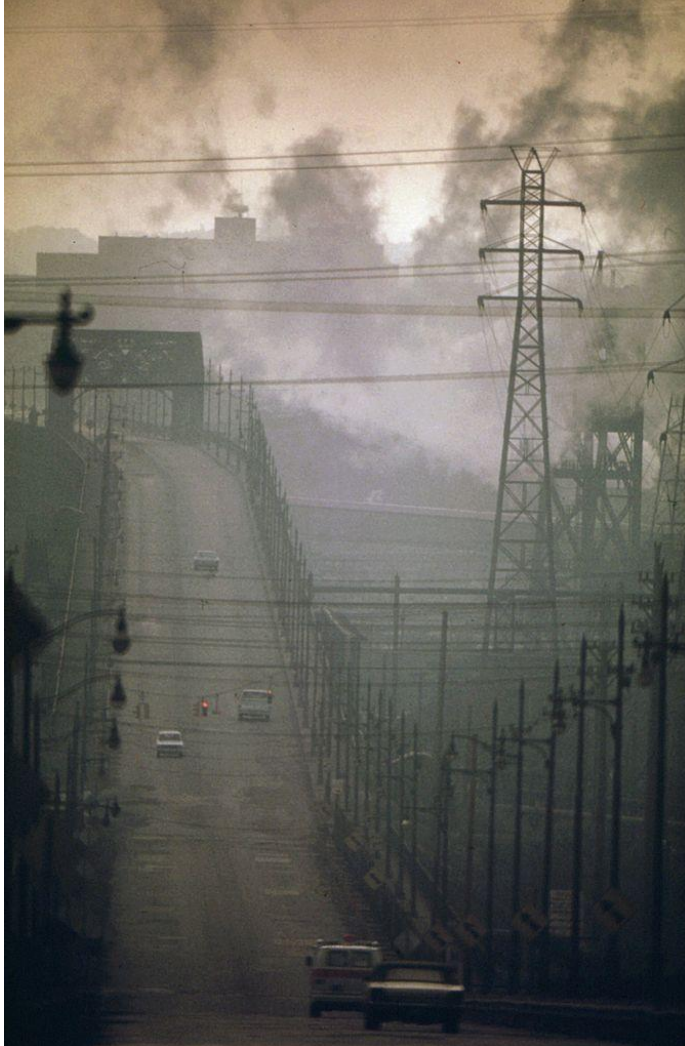
- as electron acceptors
- as **proton donors**
- as reagents for the OH^\bullet moiety exchange

WDRACs could co-exist in two different conformations:

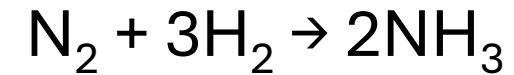
- ion-radical structure, $\text{H}_3\text{O}^+\cdots\text{OH}^\bullet$, with standard hydrogen bond
- two-center-three-electron non-classical **hemibonded** configuration, $(\text{H}_2\text{O}\cdots\text{OH}_2)^{+\bullet}$.



“Modern” nitrogen fixation: Haber-Bosch process

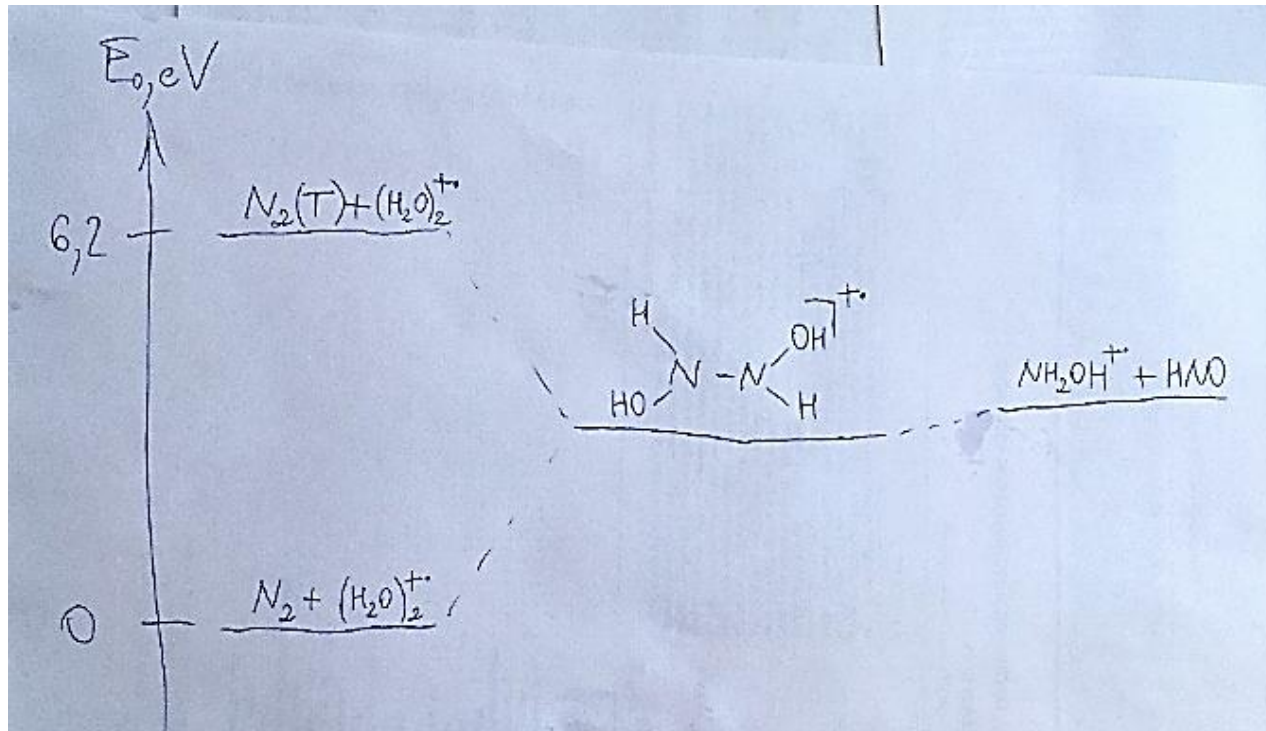


- **Haber-Bosch process** (1909) is the main industrial procedure for nitrogen fixation:



- Parameters:
 - Catalyst: Fe/FeO
 - Pressure: ~200 bar
 - Temperature: ~**500** °C

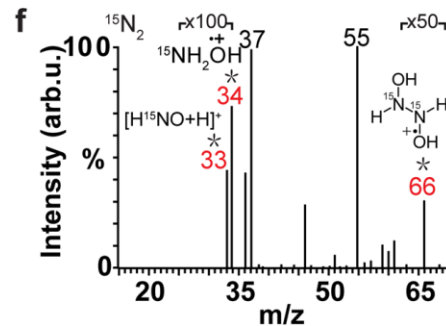
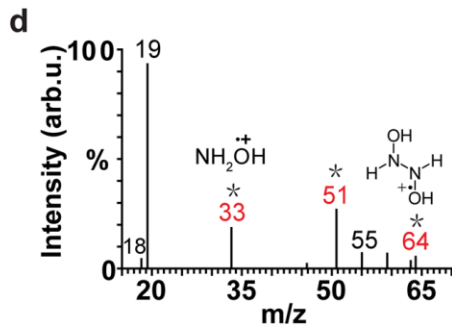
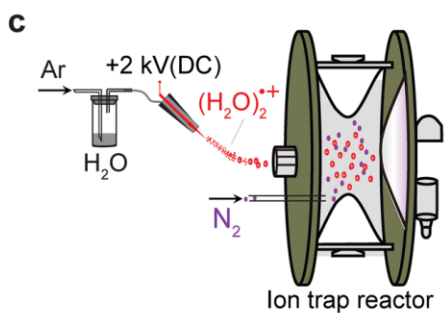
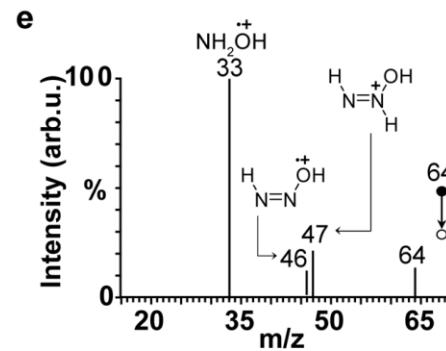
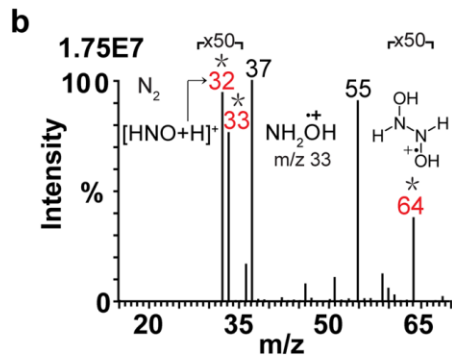
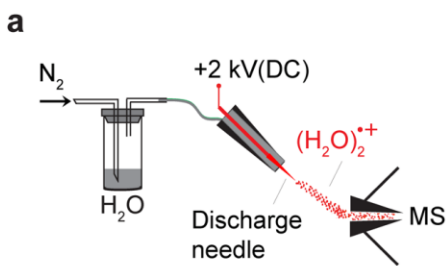
Ambient catalyst-free nitrogen fixation



- **Ambient** disproportionation reaction of N_2 with water dimer radical-cation:



Ambient catalyst-free nitrogen fixation

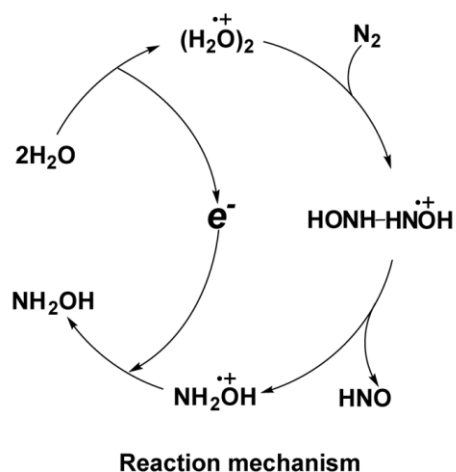


- **Ambient** disproportionation reaction of N_2 with water dimer radical-cation:

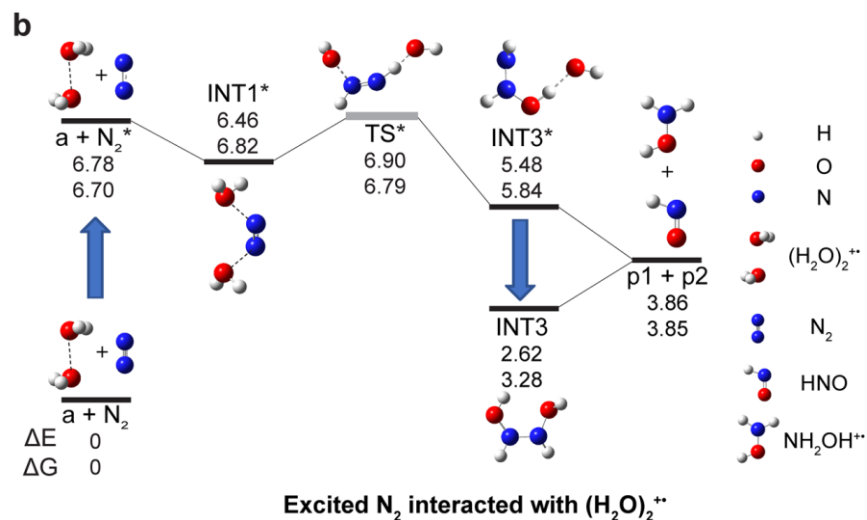


Ambient catalyst-free nitrogen fixation

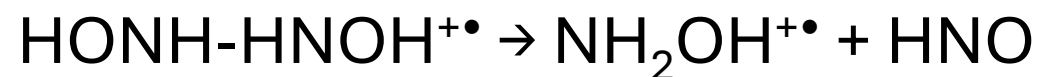
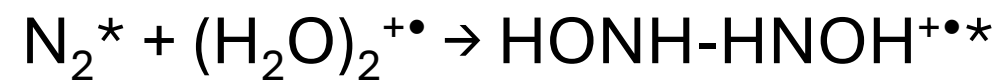
a



b

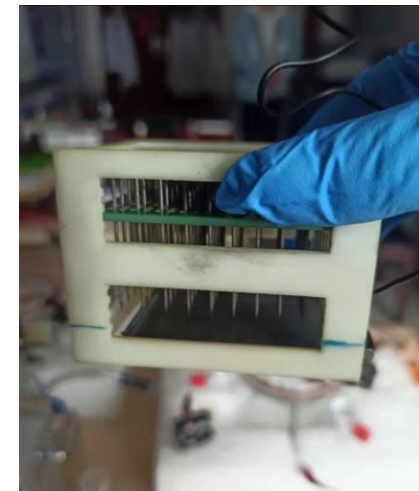
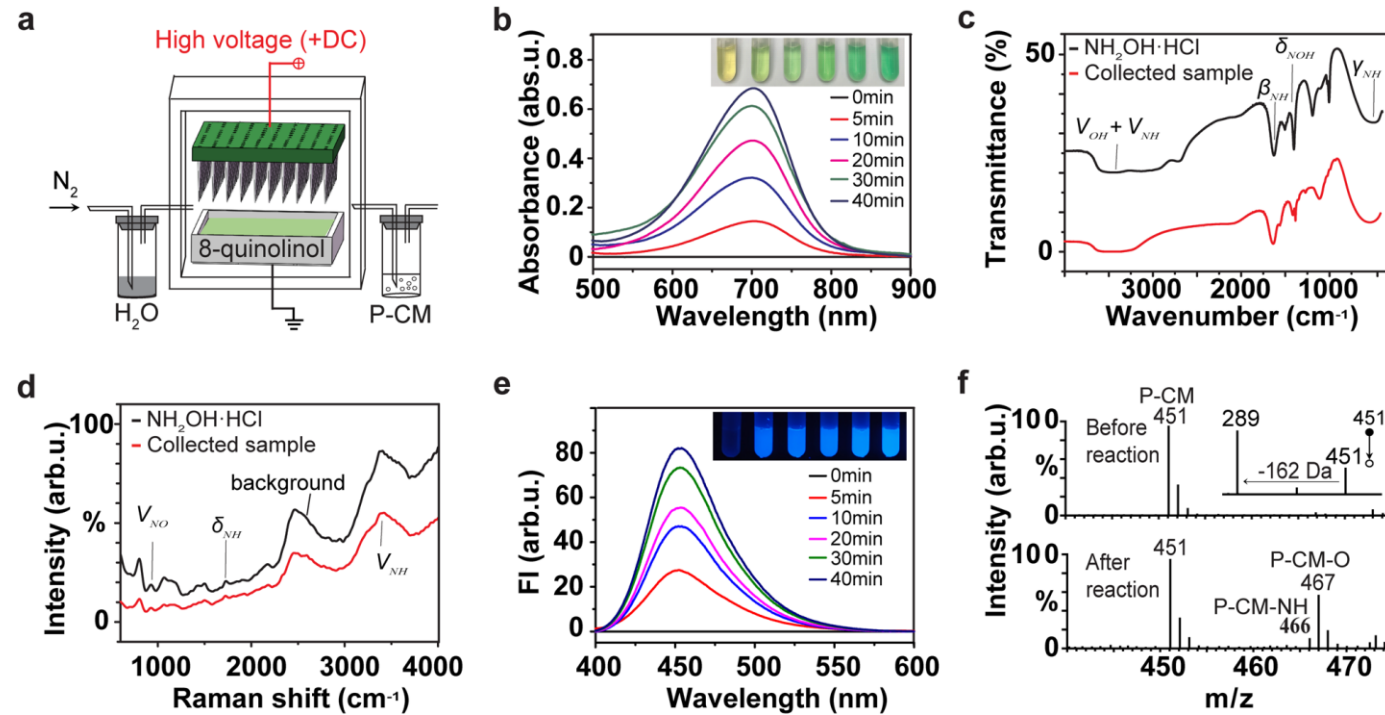
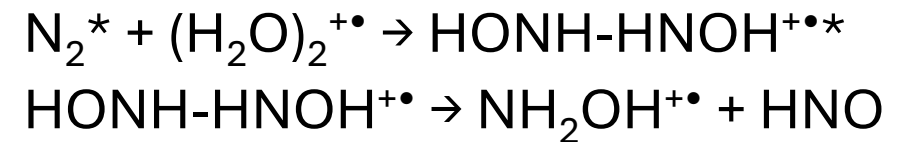


- **Ambient** disproportionation reaction of N_2 with water dimer radical cation:



Ambient catalyst-free nitrogen fixation

- Scaled-up setup and vibrational spectroscopy:



Part V. Above the ground(state)

Project Parts

- **Experimental part:**
 - Spectroscopic analysis of the long-lived intermediates in the process of ambient catalyst-free nitrogen fixation with water dimer
 - Investigation of formic acid synthesis in CO/water plasma
 - Investigation of CO₂/water & N₂O/water plasma configurations
- **Theoretical part:**
 - Calculation of N₂ fixation by water radical-cations at CCSD(T) level
 - Plasma parameters estimation by numerical methods
- **Industrial part:**
 - Contact with hydroxylamine/nitroxyl producers
 - Obtaining the grant of a patent
 - Industrial project detailing

Project Timeline

Time		Field		
		Experimental	Theoretical	Industrial
2024	Q1	Building of a new plasma setup with optical profiling	Calculation of nitrogen fixation by water dimer radical-cation at CCSD(T) level	General market analysis
	Q2			Gathering of leads and ideas
	Q3	The new setup optimization	Going beyond CC-methods: application of Weizmann-1 scheme, iFCI, and MBE-FCI on (H ₂ O) ₂ ⁺⁺	SWOT matrix analysis
	Q4	Investigation of water-plasma parameters		Contact with hydroxylamine/nitroxyl producers, wholesalers, and consumers in South Central China
2025	Q1	Investigation of methanol-plasma parameters & CH ₃ OH dimer production	Plasma parameters estimation by numerical methods	Contact with hydroxylamine/nitroxyl producers, wholesalers, and consumers in East China
	Q2	Investigation of MTBE-plasma parameters & MTBE dimer production		
	Q3	Investigation of formic acid synthesis in CO/water plasma	Calculation of formic acid synthesis in plasma at CCSD(T) level	Creation of a launch strategy
	Q4	Investigation of CO ₂ /water & N ₂ O/water plasma configurations		Initiating the process of obtaining the grant of a patent
2026	Q1	Building of a new plasma reactor based on the previous findings	Calculation of the long-lived intermediates in CO ₂ /water plasma at CCSD(T) level	Getting declarations of intent (LOIs) from the potential shareholders
	Q2			
	Q3		Acquiring third-party funds	
	Q4	The reactor test & optimization		Benchmarking of recent DFT methods: SCAN, B05, and B13+ functionals

Thank you for your attention!

感谢您的关注!

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References

1. Balabin, R. M., Syunyaev, R. Z., & Karpov, S. A. (2007). Molar enthalpy of vaporization of ethanol–gasoline mixtures and their colloid state. In *Fuel* (Vol. 86, Issue 3, pp. 323–327).
2. Syunyaev, R. Z., & Balabin, R. M. (2007). Frequency Dependence of Oil Conductivity at High Pressure. In *Journal of Dispersion Science and Technology* (Vol. 28, Issue 3, p. 419).
3. Balabin, R. M., Syunyaev, R. Z., & Karpov, S. A. (2007). Quantitative Measurement of Ethanol Distribution over Fractions of Ethanol–Gasoline Fuel. In *Energy Fuels* (Vol. 21, Issue 4, pp. 2460–2465). American Chemical Society (ACS). <https://doi.org/10.1021/ef070081l>
4. Balabin, R. M., Safieva, R. Z., & Lomakina, E. I. (2007). Comparison of linear and nonlinear calibration models based on near infrared (NIR) spectroscopy data for gasoline properties prediction. In *Chemometrics and Intelligent Laboratory Systems* (Vol. 88, Issue 2, pp. 183–188). <https://doi.org/10.1016/j.chemolab.2007.04.006>
5. Balabin, R. M., & Safieva, R. Z. (2007). Capabilities of near Infrared Spectroscopy for the Determination of Petroleum Macromolecule Content in Aromatic Solutions. In *Journal of Near Infrared Spectroscopy* (Vol. 15, Issue 6, pp. 343–349). SAGE. <https://doi.org/10.1255/jnirs.749>
6. Balabin, R. M. (2008). Dispersed Structure of Ethanol-Gasoline Fuel According to Dynamic Light Scattering Method. In *Journal of Dispersion Science and Technology* (Vol. 29, Issue 3, pp. 457–463). Informa UK Limited. <https://doi.org/10.1080/01932690701718925>
7. Balabin, R. M., & Syunyaev, R. Z. (2008). Petroleum resins adsorption onto quartz sand: Near infrared (NIR) spectroscopy study. In *Journal of Colloid and Interface Science* (Vol. 318, Issue 2, pp. 167–174). Elsevier BV. <https://doi.org/10.1016/j.jcis.2007.10.045>
8. Balabin, R. M., & Safieva, R. Z. (2008). Gasoline classification by source and type based on near infrared (NIR) spectroscopy data. In *Fuel* (Vol. 87, Issue 7, pp. 1096–1101).
9. Balabin, R. M., Safieva, R. Z., & Lomakina, E. I. (2008). Wavelet neural network (WNN) approach for calibration model building based on gasoline near infrared (NIR) spectra. In *Chemometrics and Intelligent Laboratory Systems* (Vol. 93, Issue 1, pp. 58–62). Elsevier BV. <https://doi.org/10.1016/j.chemolab.2008.04.003>
10. Balabin, R. M., & Safieva, R. Z. (2008). Motor oil classification by base stock and viscosity based on near infrared (NIR) spectroscopy data. In *Fuel* (Vol. 87, Issue 12, p. 2745).
11. Balabin, R. M. (2008). Intermolecular dispersion interactions of normal alkanes with rare gas atoms: van der Waals complexes of n-pentane with helium, neon, and argon. In *Chemical Physics* (Vol. 352, Issues 1–3, pp. 267–275). Elsevier BV. <https://doi.org/10.1016/j.chemphys.2008.06.015>
12. Balabin, R. M. (2008). Enthalpy difference between conformations of normal alkanes: Intramolecular basis set superposition error (BSSE) in the case of n-butane and n-hexane. In *The Journal of Chemical Physics* (Vol. 129, Issue 16, p. 164101). AIP Publishing. <https://doi.org/10.1063/1.2997349>
13. Syunyaev, R. Z., & Balabin, R. M. (2008). Polarization of Fluorescence of Asphaltene Containing Systems. In *Journal of Dispersion Science Technology* (Vol. 29, Issue 10, p. 1505).
14. Balabin, R. M. (2009). Enthalpy Difference between Conformations of Normal Alkanes: Raman Spectroscopy Study of n-Pentane and n-Butane. In *The Journal of Physical Chemistry A* (Vol. 113, Issue 6, pp. 1012–1019). American Chemical Society (ACS). <https://doi.org/10.1021/jp809639s>
15. Syunyaev, R. Z., Balabin, R. M., Akhatov, I. S., & Safieva, J. O. (2009). Adsorption of Petroleum Asphaltenes onto Reservoir Rock Sands Studied by Near-Infrared (NIR) Spectroscopy. In *Energy Fuels* (Vol. 23, Issue 3, pp. 1230–1236). ACS. <https://doi.org/10.1021/ef8006068>
16. Balabin, R. M. (2009). Polar (Acyclic) Isomer of Formic Acid Dimer: Gas-Phase Raman Spectroscopy Study and Thermodynamic Parameters. In *The Journal of Physical Chemistry A* (Vol. 113, Issue 17, pp. 4910–4918). American Chemical Society (ACS). <https://doi.org/10.1021/jp9002643>
17. Balabin, R. M., & Lomakina, E. I. (2009). Neural network approach to quantum-chemistry data: Accurate prediction of density functional theory energies. In *The Journal of Chemical Physics* (Vol. 131, Issue 7, p. 074104). AIP Publishing. <https://doi.org/10.1063/1.3206326>
18. Balabin, R. M., Safieva, R. Z., & Lomakina, E. I. (2008). Universal technique for optimization of neural network training parameters: gasoline near infrared data example. In *Neural Computing and Applications* (Vol. 18, Issue 6, pp. 557–565). Springer. <https://doi.org/10.1007/s00521-008-0213-3>
19. Balabin, R. M. (2009). Conformational equilibrium in glycine: Focal-point analysis and ab initio limit. In *Chemical Physics Letters* (Vol. 479, Issues 4–6, pp. 195–200).
20. Balabin, R. M. (2009). Tautomeric equilibrium and hydrogen shifts in tetrazole and triazoles: Focal-point analysis and ab initio limit. In *J Chem Phys* (Vol. 131, Issue 15, p. 154307).
21. Balabin, R. M., & Safieva, R. Z. (2011). Biodiesel classification by base stock type (vegetable oil) using near infrared spectroscopy data. In *Analytica Chimica Acta* (Vol. 689, Issue 2, pp. 190–197). <https://doi.org/10.1016/j.aca.2011.01.041>

References

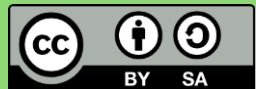
22. Chingin, K., Balabin, R. M., Barylyuk, K., Chen, H., Frankevich, V., & Zenobi, R. (2010). Rhodamines in the gas phase: cations, neutrals, anions, and adducts with metal cations. In *Physical Chemistry Chemical Physics* (Vol. 12, Issue 37, p. 11710). RSC. <https://doi.org/10.1039/c000807a>
23. Balabin, R. M. (2010). The identification of the two missing conformers of gas-phase alanine: a jet-cooled Raman spectroscopy study. In *Physical Chemistry Chemical Physics* (Vol. 12, Issue 23, p. 5980). Royal Society of Chemistry (RSC). <https://doi.org/10.1039/b924029b>
24. Chingin, K., Balabin, R. M., Frankevich, V., Chen, H., Barylyuk, K., Nieckarz, R., Fedorov, A., & Zenobi, R. (2010). Optical properties of protonated Rhodamine 19 isomers in solution and in the gas phase. In *Physical Chemistry Chemical Physics* (Vol. 12, Issue 42, p. 14121). <https://doi.org/10.1039/c0cp00482k>
25. Barylyuk, K. V., Chingin, K., Balabin, R. M., & Zenobi, R. (2010). Fragmentation of benzylpyridinium “thermometer” ions and its effect on the accuracy of internal energy calibration. In *The Journal of the American Society for Mass Spectrometry* (Vol. 21, Issue 1, pp. 172–177). ACS. <https://doi.org/10.1016/j.jasms.2009.09.023>
26. Balabin, R. M. (2009). Conformational Equilibrium in Glycine: Experimental Jet-Cooled Raman Spectrum. In *The Journal of Physical Chemistry Letters* (Vol. 1, Issue 1, pp. 20–23).
27. Schmid, T., Sebesta, A., Stadler, J., Opilik, L., Balabin, R. M., & Zenobi, R. (2010). Tip-enhanced Raman spectroscopy and related techniques in studies of biological materials. In J. Dubowski, D. B. Geohegan, & F. Träger (Eds.), *SPIE* (Vol. 7586, p. 758603). <https://doi.org/10.1117/12.845471>
28. Chingin, K., Frankevich, V., Balabin, R. M., Barylyuk, K., Chen, H., Wang, R., & Zenobi, R. (2010). Direct Access to Isolated Biomolecules under Ambient Conditions. In *Angewandte Chemie* (Vol. 49, Issue 13, pp. 2358–2361). Wiley. <https://doi.org/10.1002/anie.200906213>
29. Balabin, R. M. (2010). Boryl Substitution of Acetaldehyde Makes It an Enol: Inconsistency between Gn/CBS and Ab Initio/DFT Data. In *The Journal of Physical Chemistry A* (Vol. 114, Issue 10, pp. 3698–3702). American Chemical Society (ACS). <https://doi.org/10.1021/jp911802v>
30. Balabin, R. M. (2010). Communications: Intramolecular basis set superposition error as a measure of basis set incompleteness: Can one reach the basis set limit without extrapolation? In *The Journal of Chemical Physics* (Vol. 132, Issue 21, p. 211103). AIP. <https://doi.org/10.1063/1.3430647>
31. Balabin, R. M. (2010). Communications: Is quantum chemical treatment of biopolymers accurate? Intramolecular basis set superposition error (BSSE). In *The Journal of Chemical Physics* (Vol. 132, Issue 23, p. 231101). AIP. <https://doi.org/10.1063/1.3442466>
32. Balabin, R. M. (2010). Reply to “Comment on ‘Enthalpy Difference between Conformations of Normal Alkanes: Raman Spectroscopy Study of n-Pentane and n-Butane.’” In *The Journal of Physical Chemistry A* (Vol. 114, Issue 24, pp. 6729–6730). ACS. <https://doi.org/10.1021/jp103852d>
33. Balabin, R. M., Safieva, R. Z., & Lomakina, E. I. (2010). Gasoline classification using near infrared (NIR) spectroscopy data: Comparison of multivariate techniques. In *Analytica Chimica Acta* (Vol. 671, Issues 1–2, pp. 27–35). Elsevier BV. <https://doi.org/10.1016/j.aca.2010.05.013>
34. Opilik, L., Schmid, T., Stadler, J., Balabin, R. M., & Zenobi, R. (2010). Nanoscale Chemical Analysis of Cell Membrane Constituents Using Tip-Enhanced Raman Spectroscopy. In *AIP Conference Proceedings* (pp. 1271–1272). AIP. <https://doi.org/10.1063/1.3482420>
35. Amantonico, A., Urban, P. L., Fagerer, S. R., Balabin, R. M., & Zenobi, R. (2010). Single-Cell MALDI-MS as an Analytical Tool for Studying Intrapopulation Metabolic Heterogeneity. In *Analytical Chemistry* (Vol. 82, Issue 17, p. 7394). ACS. <https://doi.org/10.1021/ac1015326>
36. Zhu, L., Hu, Z., Gamez, G., Law, W. S., Chen, H., Yang, S., Chingin, K., Balabin, R. M., Wang, R., Zhang, T., & Zenobi, R. (2010). Simultaneous sampling of volatile and non-volatile analytes in beer for fast fingerprinting by extractive electrospray ionization mass spectrometry. In *Analytical and Bioanalytical Chemistry* (Vol. 398, Issue 1, pp. 405–413).
37. Balabin, R. M. (2010). The First Step in Glycine Solvation: The Glycine–Water Complex. In *The Journal of Physical Chemistry B* (Vol. 114, Issue 46, pp. 15075–15078).
38. Balabin, R. M., & Lomakina, E. I. (2011). Support vector machine regression (LS-SVM)—an alternative to artificial neural networks (ANNs) for the analysis of quantum chemistry data? In *Physical Chemistry Chemical Physics* (Vol. 13, Issue 24, p. 11710). RSC. <https://doi.org/10.1039/c1cp00051a>
39. Law, W. S., Chen, H. W., Balabin, R., Berchtold, C., Meier, L., & Zenobi, R. (2010). Rapid fingerprinting and classification of extra virgin olive oil by microjet sampling and extractive electrospray ionization mass spectrometry. In *Analyst* (Vol. 135, Issue 4, p. 773) <https://doi.org/10.1039/b924156f>

References

- Balabin, R. M. (2011). Conformational equilibrium in alanine: Focal-point analysis and ab initio limit. In *Computational and Theoretical Chemistry* (Vol. 965, Issue 1, pp. 15–21).
- Barylyuk, K., Balabin, R. M., Grünstein, D., Kikkeri, R., Frankevich, V., Seeberger, P. H., & Zenobi, R. (2011). What Happens to Hydrophobic Interactions during Transfer from the Solution to the Gas Phase? The Case of Electrospray-Based Soft Ionization Methods. In *Journal of the American Society for Mass Spectrometry* (Vol. 22, Issue 7, pp. 1167–1177).
- Balabin, R. M., & Smirnov, S. V. (2011). Variable selection in near-infrared spectroscopy: Benchmarking of feature selection methods on biodiesel data. In *Analytica Chimica Acta* (Vol. 692, Issues 1–2, pp. 63–72). Elsevier BV. <https://doi.org/10.1016/j.aca.2011.03.006>
- Balabin, R. M., Lomakina, E. I., & Safieva, R. Z. (2011). Neural network (ANN) approach to biodiesel analysis: Analysis of biodiesel density, kinematic viscosity, methanol and water contents. In *Fuel* (Vol. 90, Issue 5, p. 2007). <https://doi.org/10.1016/j.fuel.2010.11.038>
- Balabin, R. M., Safieva, R. Z., & Lomakina, E. I. (2011). Near-infrared (NIR) spectroscopy for motor oil classification: From discriminant analysis to support vector machines. In *Microchemical Journal* (Vol. 98, Issue 1, pp. 121–128). Elsevier BV. <https://doi.org/10.1016/j.microc.2010.12.007>
- Balabin, R. M., & Safieva, R. Z. (2011). Near-Infrared (NIR) Spectroscopy for Biodiesel Analysis: Fractional Composition, Iodine Value, and Cold Filter Plugging Point from One Vibrational Spectrum. In *Energy Fuels* (Vol. 25, Issue 5, pp. 2373–2382). ACS. <https://doi.org/10.1021/ef200356h>
- Balabin, R. M., & Smirnov, S. V. (2011). Melamine detection by mid- and near-infrared (MIR/NIR) spectroscopy: A quick and sensitive method for dairy products analysis. In *Talanta* (Vol. 85, Issue 1, p. 562). <https://doi.org/10.1016/j.talanta.2011.04.026>
- Chingin, K., Balabin, R. M., Frankevich, V., Barylyuk, K., Nieckarz, R., Sagulenko, P., & Zenobi, R. (2011). Absorption of the green fluorescent protein chromophore anion in the gas phase studied by a combination of FTICR mass spectrometry with laser-induced photodissociation spectroscopy. In *International Journal of Mass Spectrometry* (Vol. 306, Issues 2–3, pp. 241–245). Elsevier BV. <https://doi.org/10.1016/j.ijms.2011.01.014>
- Likhatsky, V. V., Balabin, R. M., & Syunyaev, R. Z. (2011). Calculation of Dipole Moment of Fractal Asphaltene Cluster. In *Journal of Dispersion Science and Technology* (Vol. 32, Issue 10, pp. 1502–1508). Informa UK Limited. <https://doi.org/10.1080/01932691.2010.516129>
- Balabin, R. M., & Lomakina, E. I. (2011). Support vector machine regression (SVR/LS-SVM)—an alternative to neural networks (ANN) for analytical chemistry? Comparison of nonlinear methods on near infrared (NIR) spectroscopy data. In *The Analyst* (Vol. 136, Issue 8, p. 1703). Royal Society of Chemistry (RSC). <https://doi.org/10.1039/c0an00387e>
- Balabin, R. M., Syunyaev, R. Z., Schmid, T., Stadler, J., Lomakina, E. I., & Zenobi, R. (2010). Asphaltene Adsorption onto an Iron Surface: Combined Near-Infrared (NIR), Raman, and AFM Study of the Kinetics, Thermodynamics, and Layer Structure. In *Energy Fuels* (Vol. 25, Issue 1, pp. 189–196).
- Balabin, R. M. (2011). On the relation between basis set convergence and electron correlation: a critical test for modern ab initio quantum chemistry on a “mindless” data set. In *Structural Chemistry* (Vol. 22, Issue 5, pp. 1047–1051). Springer. <https://doi.org/10.1007/s11224-011-9793-0>
- Zenobi, R., Schmid, T., Syunyaev, R. Z., & Balabin, R. M. (2011). Physical chemistry of acridine adsorption onto gold surface: the influence of nanostructure as revealed by near-infrared and tip-enhanced Raman spectroscopy (TERS). In *Physical Chemistry of Interfaces and Nanomaterials X* (p. 25). *Physical Chemistry of Interfaces and Nanomaterials X*.
- Balabin, R. M. (2011). The keto-enol equilibrium in substituted acetaldehydes: focal-point analysis and ab initio limit. In *Molecular Physics* (Vol. 109, Issue 19, pp. 2341–2351).
- Balabin, R. M., & Smirnov, S. V. (2012). Interpolation and extrapolation problems of multivariate regression in analytical chemistry: benchmarking the robustness on near-infrared (NIR) spectroscopy data. In *The Analyst* (Vol. 137, Issue 7, p. 1604). RSC. <https://doi.org/10.1039/c2an15972d>
- Barylyuk, K., Fritsche, L., Balabin, R. M., Nieckarz, R., & Zenobi, R. (2012). Gas-phase basicity of several common MALDI matrices measured by a simple experimental approach. In *RSC Advances* (Vol. 2, Issue 5, p. 1962). Royal Society of Chemistry (RSC). <https://doi.org/10.1039/c1ra01117k>
- Balabin, R. M. (2012). Experimental thermodynamics of free glycine conformations: the first Raman experiment after twenty years of calculations. In *Phys. Chem. Chem. Phys.* (Vol. 14, Issue 1, pp. 99–103). Royal Society of Chemistry (RSC). <https://doi.org/10.1039/c1cp20805e>
- Balabin, R. M. (2011). Enthalpy difference between conformations of normal alkanes: effects of basis set and chain length on intramolecular basis set superposition error. In *Molecular Physics* (Vol. 109, Issue 6, pp. 943–953). Informa UK Limited. <https://doi.org/10.1080/00268976.2011.558858>

References

58. Barylyuk, K., Balabin, R. M., Grünstein, D., Kikkeri, R., Frankevich, V., Seeberger, P. H., & Zenobi, R. (2011). What Happens to Hydrophobic Interactions during Transfer from the Solution to the Gas Phase? The Case of Electrospray-Based Soft Ionization Methods. In *Journal of the American Society for Mass Spectrometry* (Vol. 22, Issue 7, pp. 1167–1177).
59. Balabin, R. M., & Smirnov, S. V. (2011). Variable selection in near-infrared spectroscopy: Benchmarking of feature selection methods on biodiesel data. In *Analytica Chimica Acta* (Vol. 692, Issues 1–2, pp. 63–72). Elsevier BV. <https://doi.org/10.1016/j.aca.2011.03.006>
60. Balabin, R. M., Lomakina, E. I., & Safieva, R. Z. (2011). Neural network (ANN) approach to biodiesel analysis: Analysis of biodiesel density, kinematic viscosity, methanol and water contents. In *Fuel* (Vol. 90, Issue 5, p. 2007). Elsevier BV. <https://doi.org/10.1016/j.fuel.2010.11.038>
61. Balabin, R. M., Safieva, R. Z., & Lomakina, E. I. (2011). Near-infrared (NIR) spectroscopy for motor oil classification: From discriminant analysis to support vector machines. In *Microchemical Journal* (Vol. 98, Issue 1, pp. 121–128). Elsevier BV. <https://doi.org/10.1016/j.microc.2010.12.007>
62. Balabin, R. M., & Safieva, R. Z. (2011). Near-Infrared (NIR) Spectroscopy for Biodiesel Analysis: Fractional Composition, Iodine Value, and Cold Filter Plugging Point from One Vibrational Spectrum. In *Energy Fuels* (Vol. 25, Issue 5, pp. 2373–2382). ACS. <https://doi.org/10.1021/ef200356h>
63. Balabin, R. M., & Smirnov, S. V. (2011). Melamine detection by mid- and near-infrared (MIR/NIR) spectroscopy: A quick and sensitive method for dairy products analysis. In *Talanta* (Vol. 85, Issue 1, p. 562). Elsevier BV. <https://doi.org/10.1016/j.talanta.2011.04.026>
64. Chingin, K., Balabin, R. M., Frankevich, V., Barylyuk, K., Nieckarz, R., Sagulenko, P., & Zenobi, R. (2011). Absorption of the green fluorescent protein chromophore anion in the gas phase studied by a combination of FTICR mass spectrometry with laser-induced photodissociation spectroscopy. In *International Journal of Mass Spectrometry* (Vol. 306, Issues 2–3, pp. 241–245). Elsevier BV. <https://doi.org/10.1016/j.ijms.2011.01.014>
65. Zhang, X., Su, R., Li, J., Huang, L., Yang, W., Chingin, K., Balabin, R., Wang, J., Zhang, X., Zhu, W., Huang, K., Feng, S., & Chen, H. (2024). Efficient catalyst-free N₂ fixation by water radical cations under ambient conditions. *Nature Communications*.
66. Zhang, X., Hu, P., Duan, M., Chingin, K., Balabin, R., Zhang, X., & Chen, H. (2024). Ambient catalyst-free oxidation reactions of aromatic amines using water radical cations.
67. Balabin, R. V., Volkomirskaya, L. B., Gulevich, O. A., Krivosheev, N. V., Lyakhov, G. A., Musalev, D. N., Reznikov, A. E., Safieva, R. Z., & Semyonov, S. N. (2015). Georadar sensing from terrestrial surface and shafts: Approaches to evaluation of rock fracturing. In *Physics of Wave Phenomena*, 23 (2), 143–153. <https://doi.org/10.3103/s1541308x15020107>
68. Fischer, T. L., Bödecker, M., Schweer, S. M., Dupont, J., Lepère, V., Zehnacker-Rentien, A., Suhm, M. A., Schröder, B., Henkes, T., Andrada, D. M., Balabin, R. M., Singh, H. K., Bhattacharyya, H. P., Sarma, M., Käser, S., Töpfer, K., Vazquez-Salazar, L. I., Boittier, E. D., Meuwly, M., ... Mata, R. A. (2023). The first HyDRA challenge for computational vibrational spectroscopy. In *Physical Chemistry Chemical Physics*.
69. Zhang, X., Duan, M., Chingin, K., Balabin, R., Liu, L., Zhang, X., & Chen, H. (2025). Detection and Characterization of Water Radical Cations by Mass Spectrometry and Electron Paramagnetic Resonance Spectroscopy. In *Analytical Chemistry*.
70. Царев, А. В., Балабин, Р. М., Карпов, С. А., & Сюняев, Р. З. (2007). Оптимизация эксплуатационных и экологических свойств спирто-бензиновых топлив под действием микроволновой обработки. *Альтернативная энергетика и экология*, 8 (52), 69–74.
71. Балабин, Р. М. (2005). Создание экспресс-метода анализа показателей качества индустриального масла на основе многомерного анализа спектральных данных. *Достижения ученых XXI века: Тезисы докладов международной конференции*. Тамбов, 192–194.
72. Балабин, Р. М., & Сюняев, Р. З. (2006). Построение кривой стеклования нефти по данным диэлектрической спектроскопии. XIII Всероссийская конференция «Структура и динамика молекулярных систем. Яльчик 2006», 13, 57–60.
73. Сафиева, Р. З., Сюняев, Р. З., Абанина, Е. Н., Филатов, В. М., & Балабин, Р. М. (2011). Экспресс-анализ состава и физико-химических свойств нефтяных систем методом БИК-спектроскопии. *Наука и технологии в промышленности* 3, 101–104.
74. Balabin, R. (2013). *Vibrational spectroscopy in the study of oil systems: Development of rapid methods for the analysis of oil refining and petrochemical products*. Gubkin Uni.
75. Syunyaev, R. Z., Likhatsky, V. V., & Balabin, R. M. (2010) Simulation of Dipole Moment in Asphaltene Nanocluster. CHOPS, DBR Technology Center, Schlumberger Canada.



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