

From the Properties of Long-lived Intermediates in Mass Spectrometry to Applied Plasma Chemistry

Prof. Dr. Roman M. Balabin

East China University of Technology (ECUT)

Bond Street Holdings, Nevis



Outline

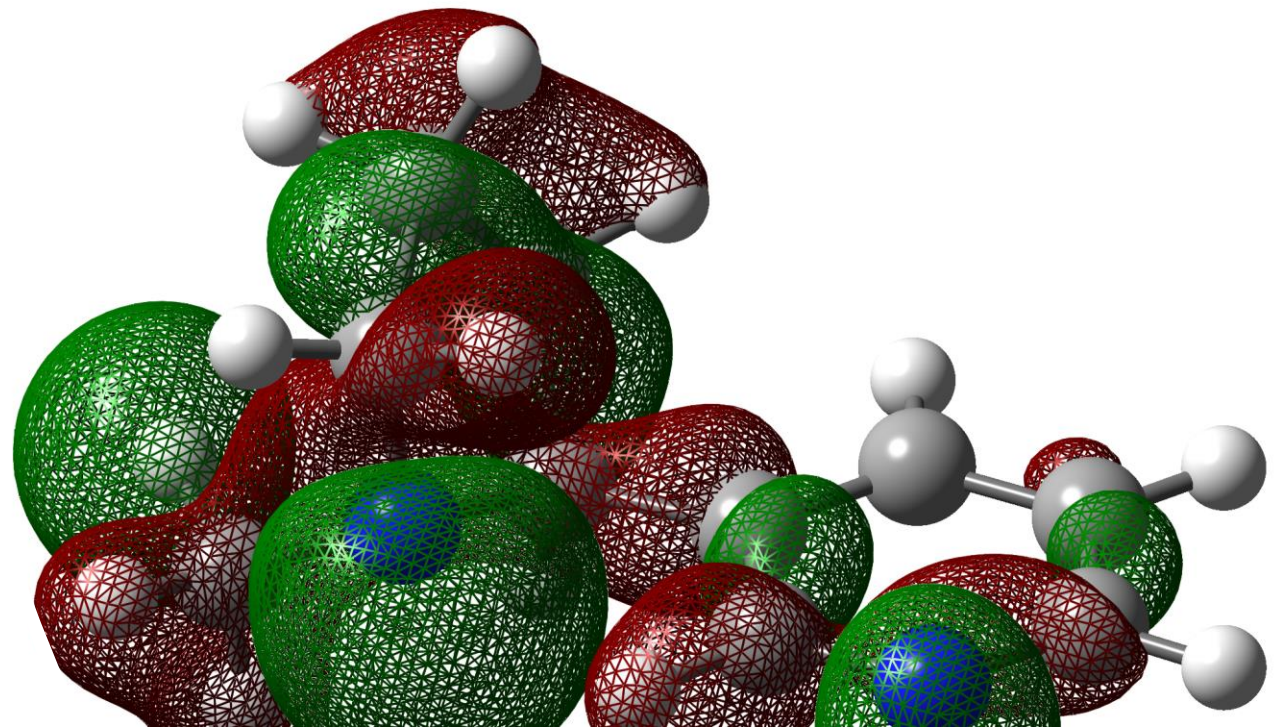
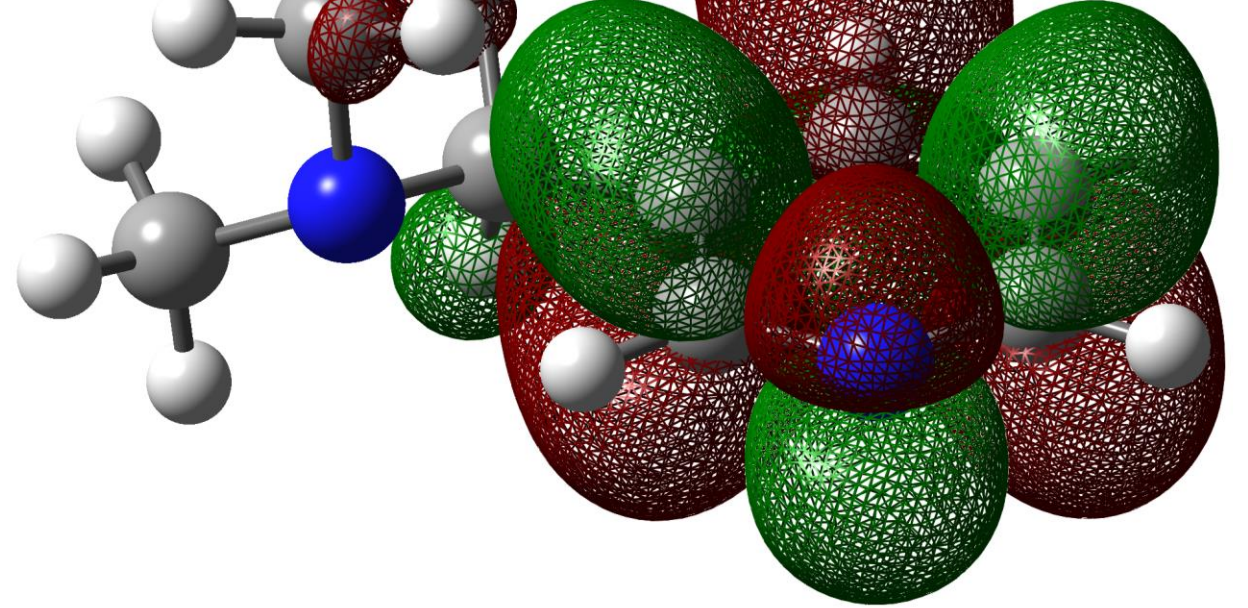
Part I. CV / Bio

Part II. Brainware Analytics

Part III. The HyDRA Challenge

Part IV. Nitrogen Fixation by
Ambient Plasma

Part V. Project Timeline



Part I. CV / Bio

Early Years: 1985–2002

- Name: **Roman M. Balabin** (*Роман Балабин*)
 - ORCID: 0000-0001-9374-1809
 - Scopus ID: 15049329900
 - ResearcherID: S-4053-2018
- Born on August 21, 1985, in the Cheryomushki (Brezhnevsky) district of **Moscow**, USSR
- Family:
 - Mother: Irina V. Balabina (25 Nov 1960, Moscow)
 - Father: Mikhail I. Balabin (Shegidevich, 19 Feb 1961, Moscow)
 - Grandfather: Izmail Yakovlevich Shegidevich (Izmaïł Jakubowicz Szegidewicz) – repressed nobleman of Polish-Tatar origin



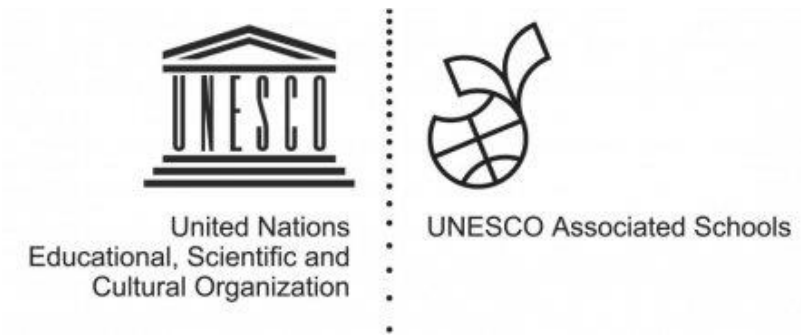
Early Years: 1985–2002

- 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



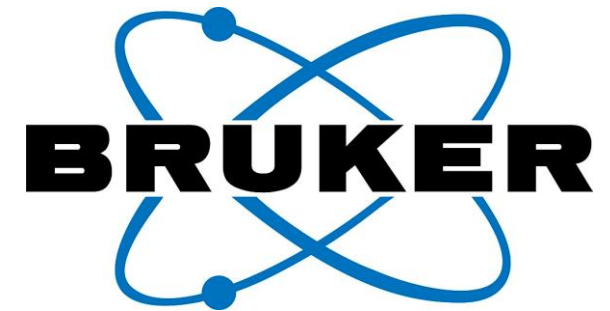
School Education

- 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, Moscow) from 2000 to 2002 – **UNESCO** Associated Schools Project Network (ASPnet)
 - Mathematics, computer science and IT
 - Diploma thesis @ **Aleksandr Giglavyj**: “Information and communication technology (ICT) market of the Baltic states” (2002)



University Years: 2002–2008

- Uni: **Gubkin Russian State University** of Oil and Gas (Moscow)
 - Faculty of Chemical Engineering and Ecology
 - Department of Organic Chemistry and Petrochemistry
 - Major / specialty: 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)
 - Nesmeyanov Institute of Organoelement Compounds



University Years: 2002–2008

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

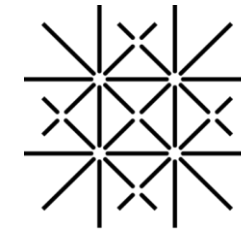
- Ruprecht Karl University of **Heidelberg** (Germany)
 - Institute of Applied Physical Chemistry
 - Group of Prof. Dr. **Michael Grunze** / Patrick Koelsch
 - Topic: sum-frequency-generation spectroscopy (SFGS) of biofilms



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 dielectric spectroscopy of macromolecular petroleum systems



Universität
Basel

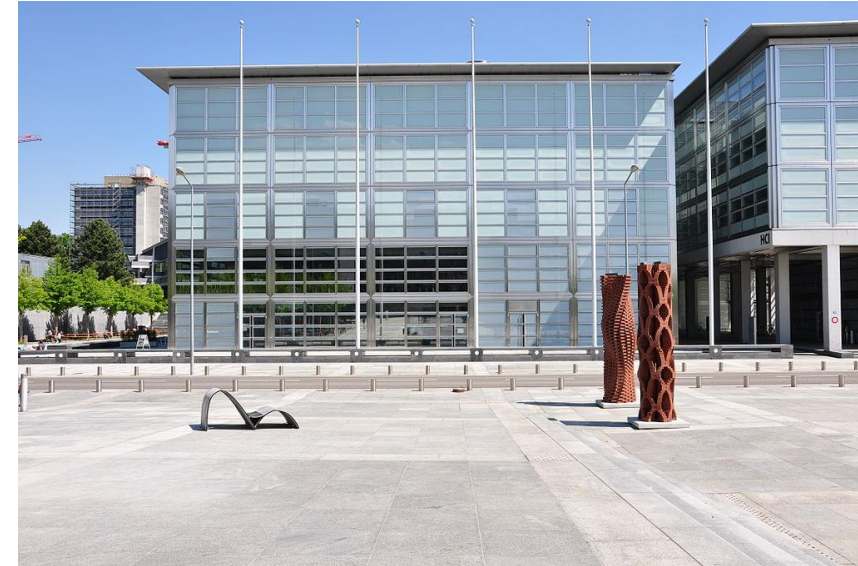
Max-Planck-Institut
für Polymerforschung

Max Planck Institute
for Polymer Research



PhD Studies: 2008–2012

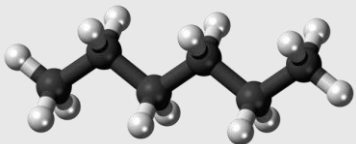
- Uni: **ETH Zurich** (Switzerland)
 - Department of Chemistry and Applied Biosciences (CHAB)
 - Group of Prof. Dr. **Renato Zenobi**
 - Vibrational spectroscopy and mass-spectrometry
 - PhD thesis: “Development of express methods for analysis of petroleum refining products and petrochemicals based on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





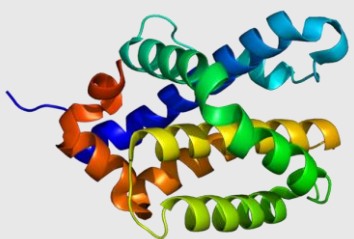
Scientific and industrial results

- 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 (2011) 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, J Colloid Interface Sci (2008) 167, JDST (2008) 1505, Energy Fuels (2009) 1230, Energy Fuels (2011) 189, JDST (2011) 1502.
 - 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 (*Computational Organic Chemistry*, 2014), 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.
 - Dral, *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)
- **Wikinews**, Miami, FL
 - Interviews with Profs. Jonathan Gruber (MIT), Clive Spash (CSIRO), Stephen Ward (UBC), Robert Costanza (UCL), Dimie Ogoina (WHO)
- **Eyewitness News (EWN)**, Johannesburg, SA

Швейцария Деловая



Part II. Brainware Analytics

Brainware Analytics: formal

- Formal: **Brainware Analytics GmbH** (Switzerland)
 - BWAN = BrainWare Analytics LLC
 - Commercial register CH-170.4.011.342-9
 - EU VAT: CHE-202.748.777
 - 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)



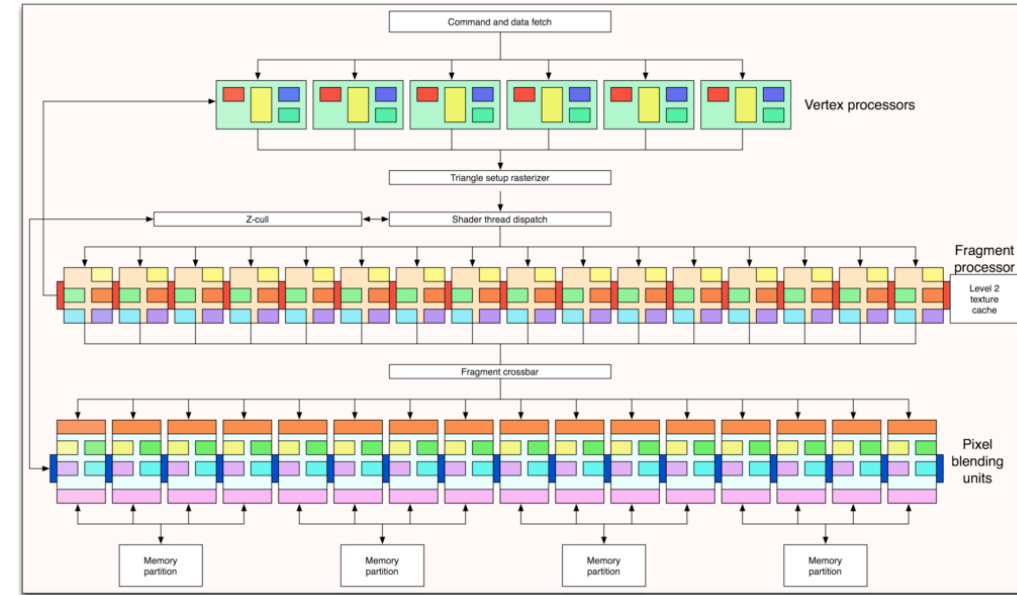
Brainware Analytics: locations

- 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)



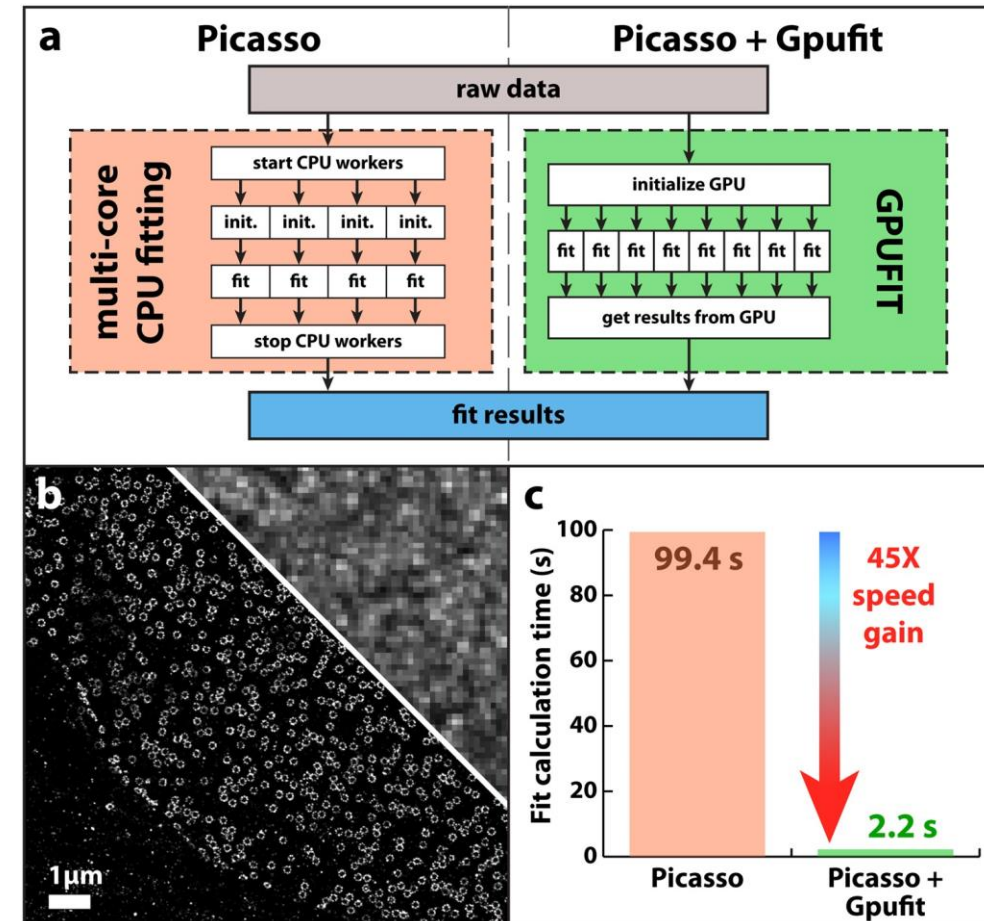
General-purpose computing on GPUs

- **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



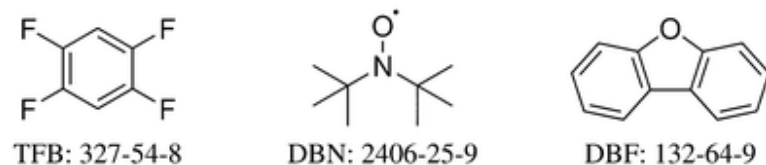
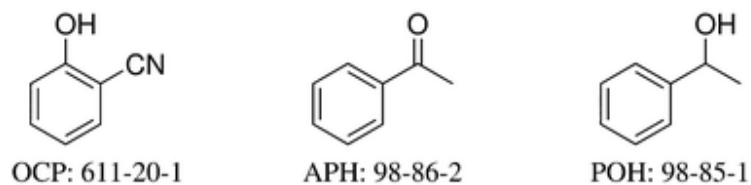
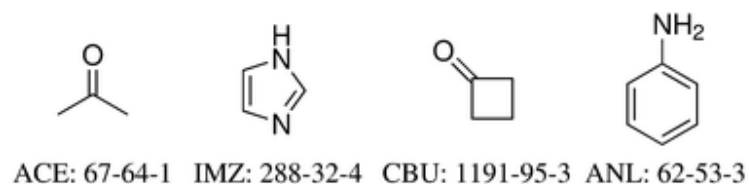
General-purpose computing on GPUs

- **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**



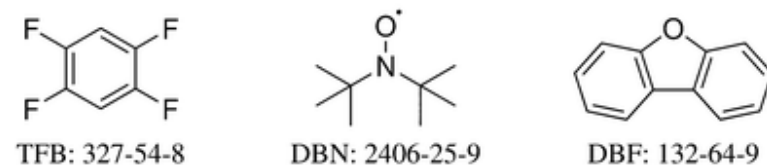
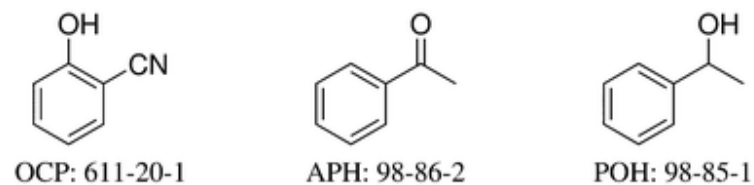
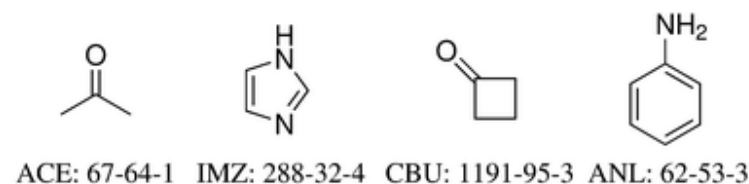
Part III. The HyDRA Challenge

The HyDRA Challenge: 2021



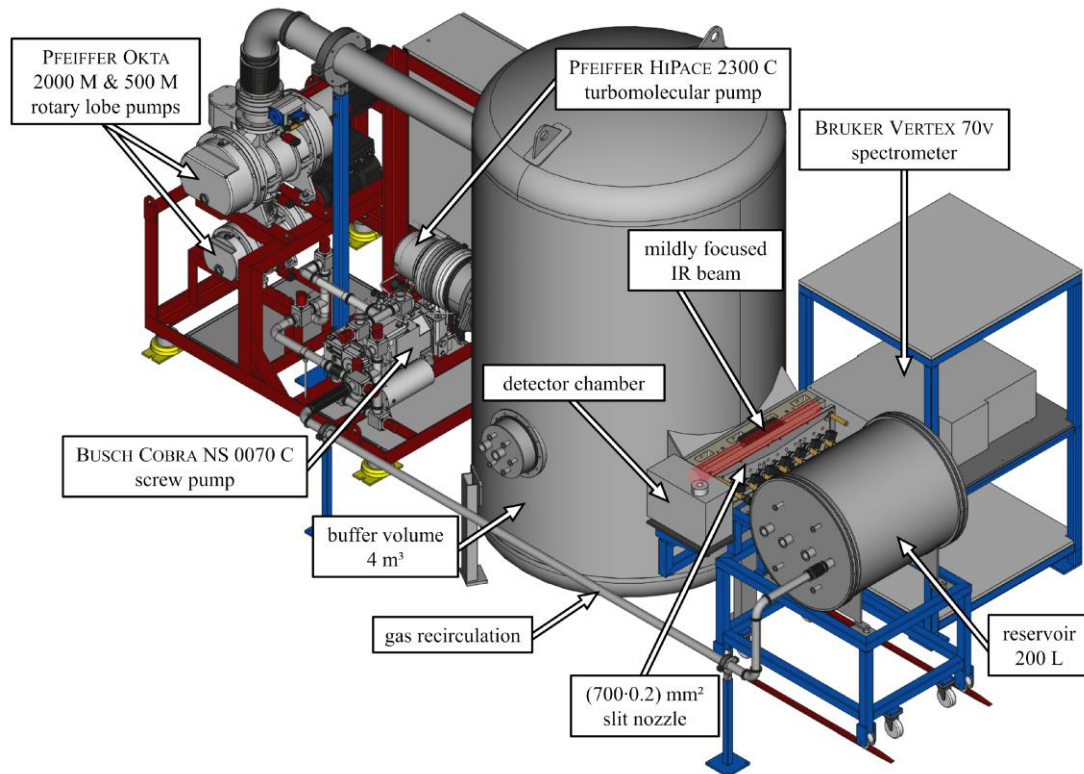
- **Hydrate Donor Redshift Anticipation (HyDRA)** blind challenge for the microhydration
- Organizers:
 - University of Göttingen / Paris-Saclay University
 - Prof. Dr. **Ricardo Mata** (theor) / Prof. Dr. **Anne Zehnacker-Rentien** (exp)
- Ten complexes of organic molecules with water
- No experimental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

The HyDRA Challenge: 2021



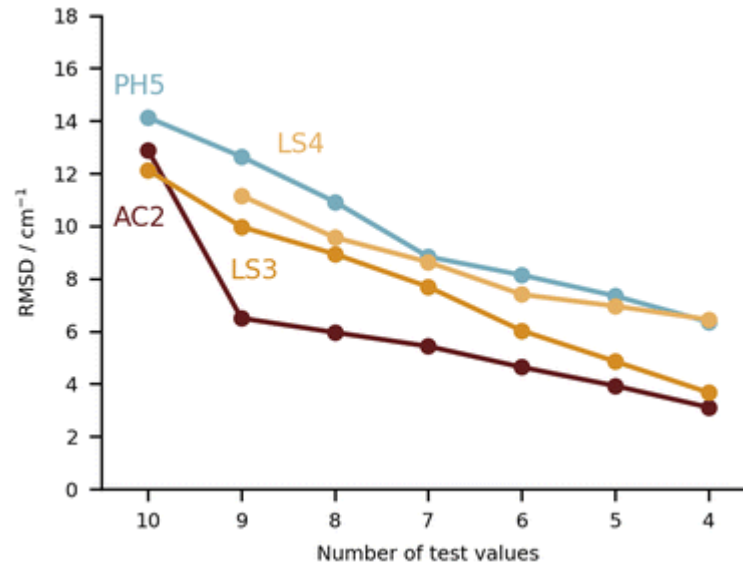
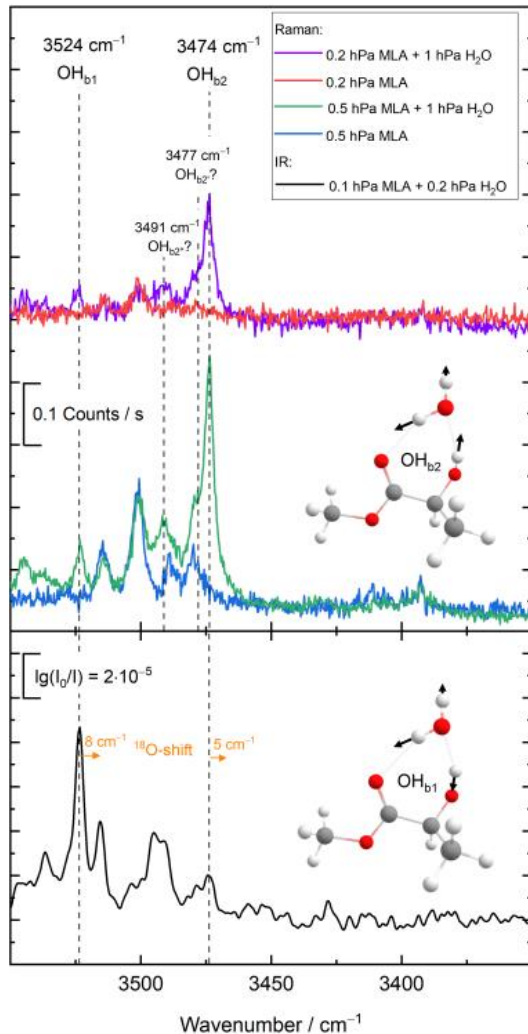
- The role of theory in understanding hydration is multifaceted:
 - Helps to **assign** the experimental spectral data
 - Could even replace experiment (to some extent)
- A need for **unbiased** tests of different predictive theoretical approaches by experiment

The HyDRA Challenge: 2023



- Submitted:
 - 18 models from 12 groups
 - mostly DFT
- Three (3) best models were selected
- Model **LS4** based on a novel DFT learning strategy that included water geometrical parameters is among **top-3**
- My idea: PBE0-D3BJ/aVT(Q)Z adjusted with a five-parameter regression function
 - Good for GPU-based calculations

The HyDRA Challenge: 2023



- Submitted:
 - 18 models from 12 groups
 - Mostly DFT
- Three (3) best models were selected by the jury
- Model **LS4** based on a novel DFT learning strategy that included water geometrical parameters is among **top-3**
- My idea: PBE0-D3BJ/aVT(Q)Z adjusted with a five-parameter regression function

Part IV. Nitrogen Fixation by Ambient Plasma

The Project

- **Experimental part:**

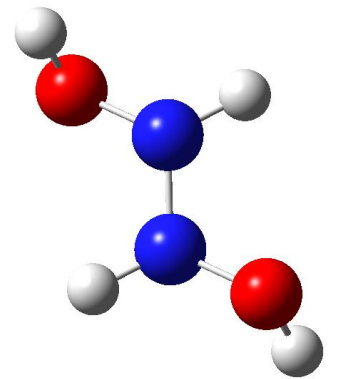
- Spectroscopic analysis of the long-lived intermediates in the process of ambient catalyst-free nitrogen fixation with water dimer
- Investigation of formic acid synthesis in CO/water plasma
- Investigation of CO₂/water & N₂O/water plasma configurations

- **Theoretical part:**

- Calculation of N₂ fixation by water radical-cations at CCSD(T) level
- Plasma parameters estimation by numerical methods

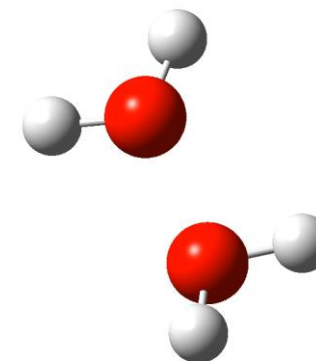
- **Industrial part:**

- Contact with hydroxylamine/nitroxyl producers
- Obtaining the grant of a patent
- Industrial project detailing

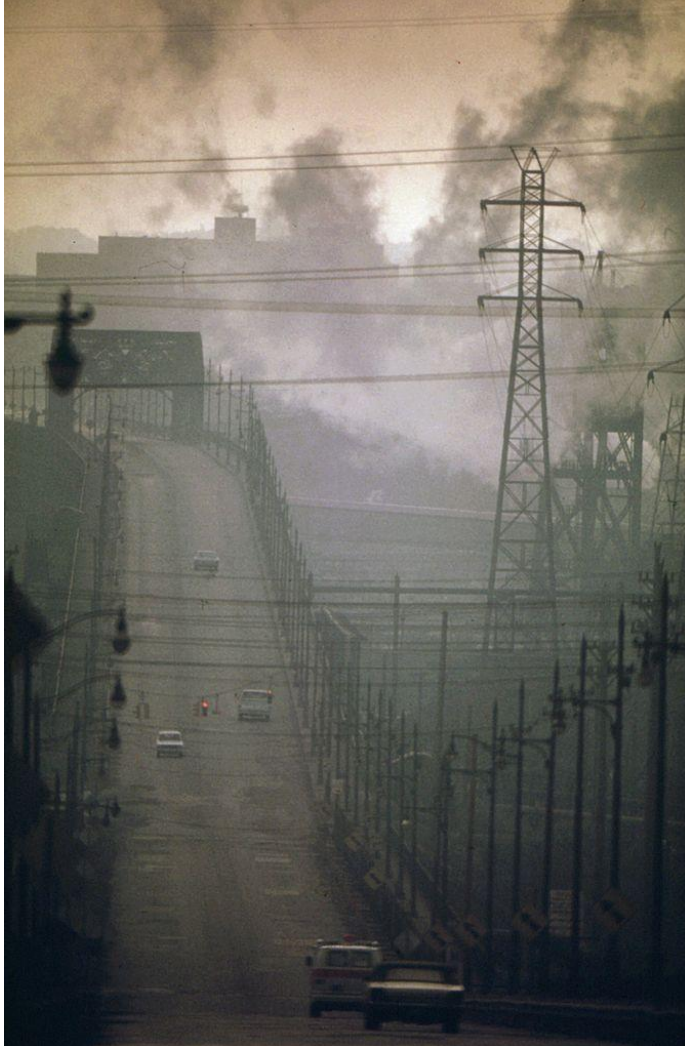


WDRAC: Water dimer radical-cation

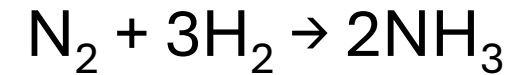
- The WDRACs, $(\text{H}_2\text{O})_2^{+\bullet}$, react with organic substances in three rather different ways:
 - as electron acceptors
 - as **proton donors**
 - as reagents for the OH^\bullet moiety exchange
- WDRACs could co-exist in two different conformations:
 - ion-radical structure, $\text{H}_3\text{O}^+\cdots\text{OH}^\bullet$, 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

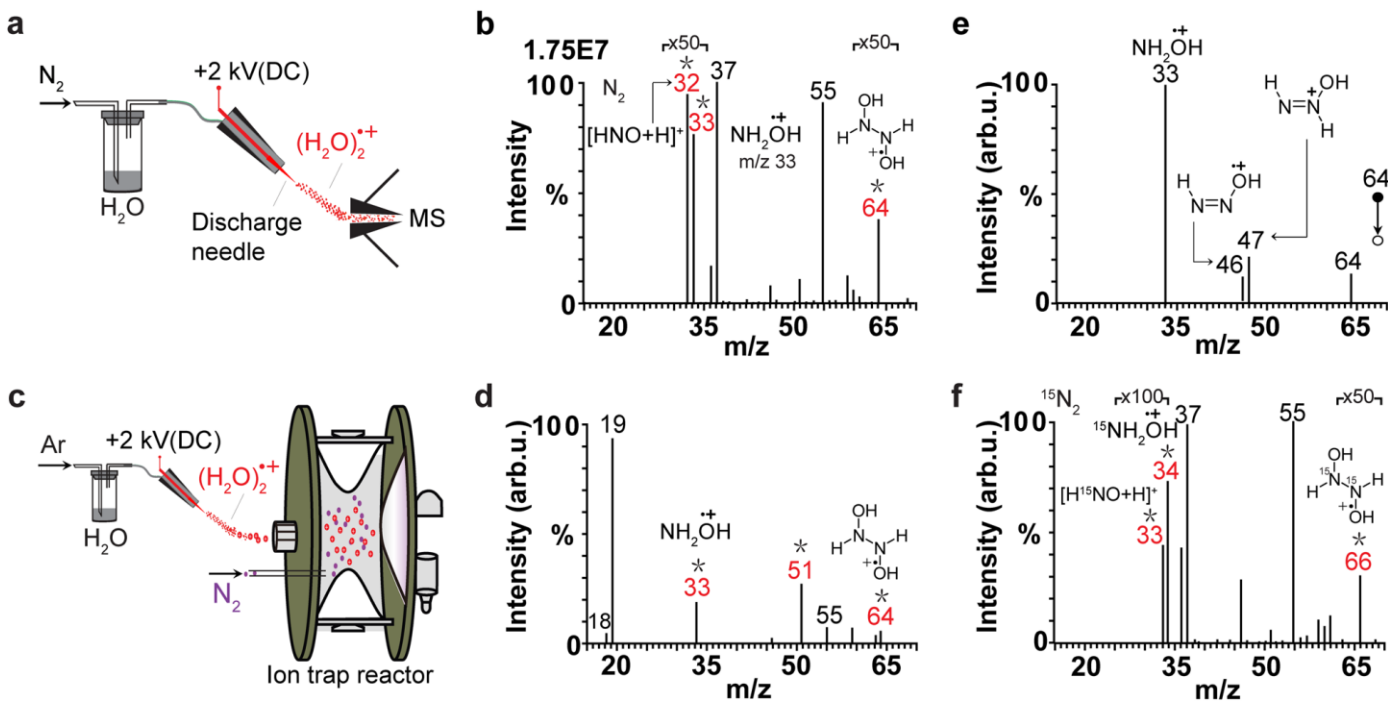


- **Haber-Bosch process** (1909) is the main industrial procedure for nitrogen fixation:



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

Ambient catalyst-free nitrogen fixation

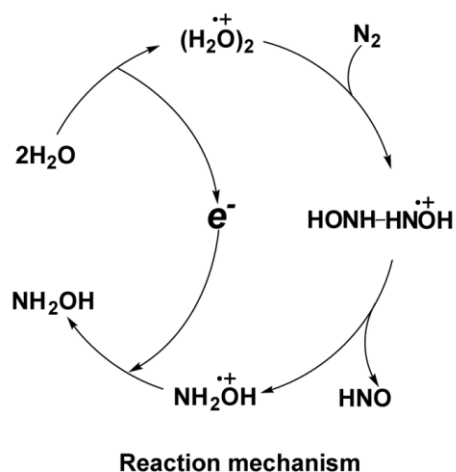


- **Ambient** disproportionation reaction of N_2 with water dimer radical-cation:

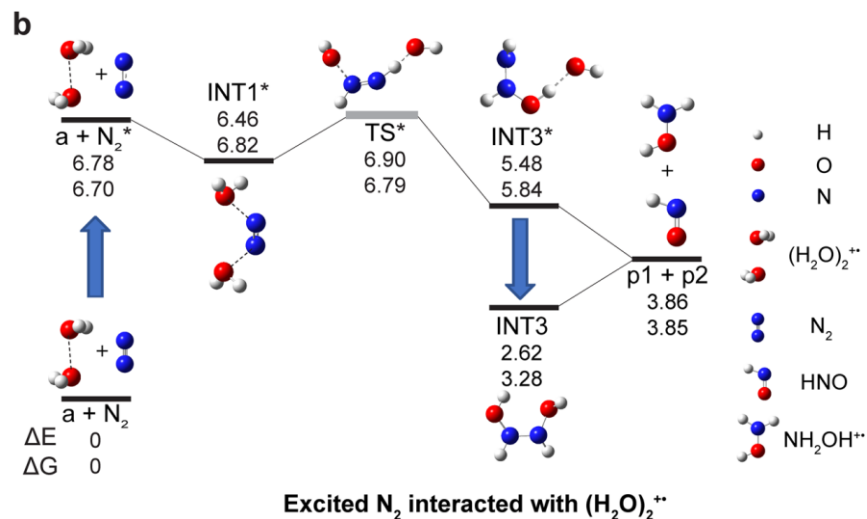


Ambient catalyst-free nitrogen fixation

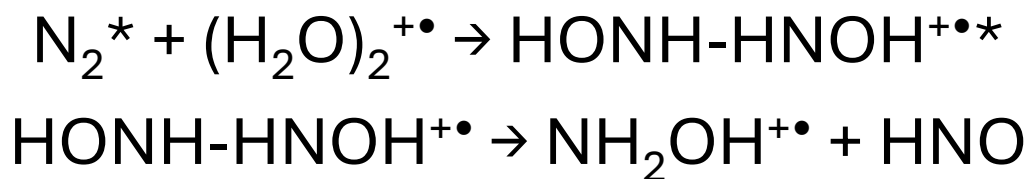
a



b

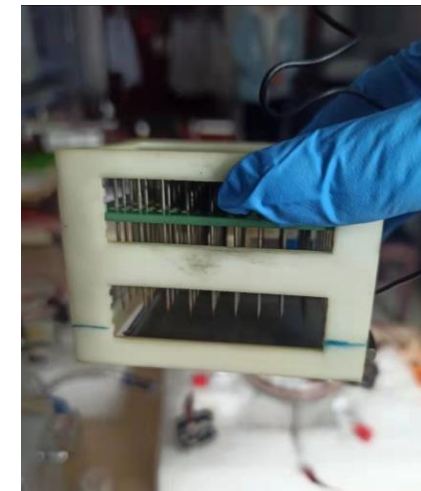
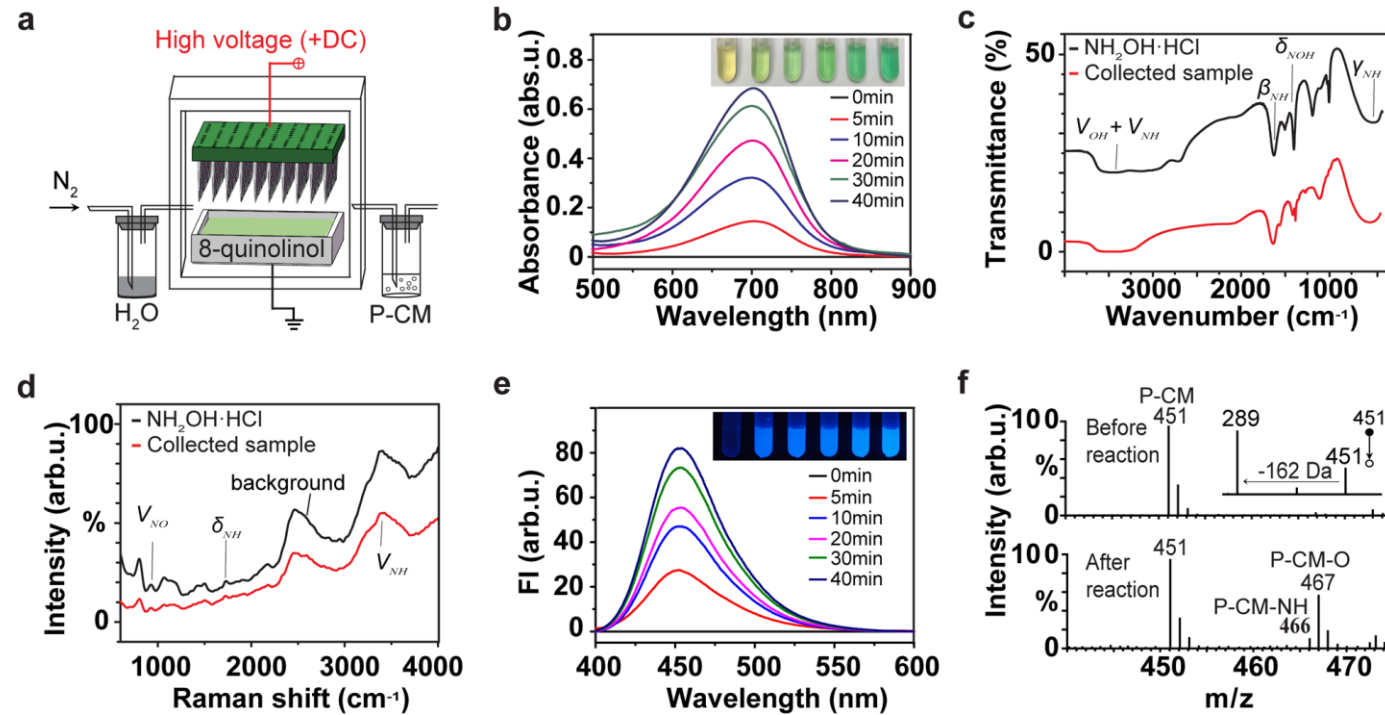
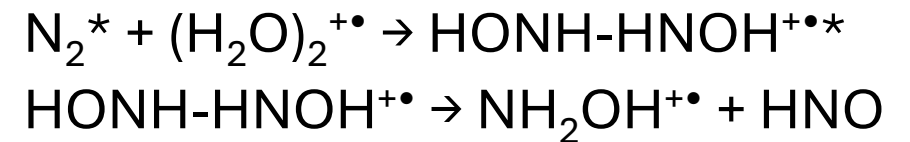


- **Ambient** disproportionation reaction of N_2 with water dimer radical cation:

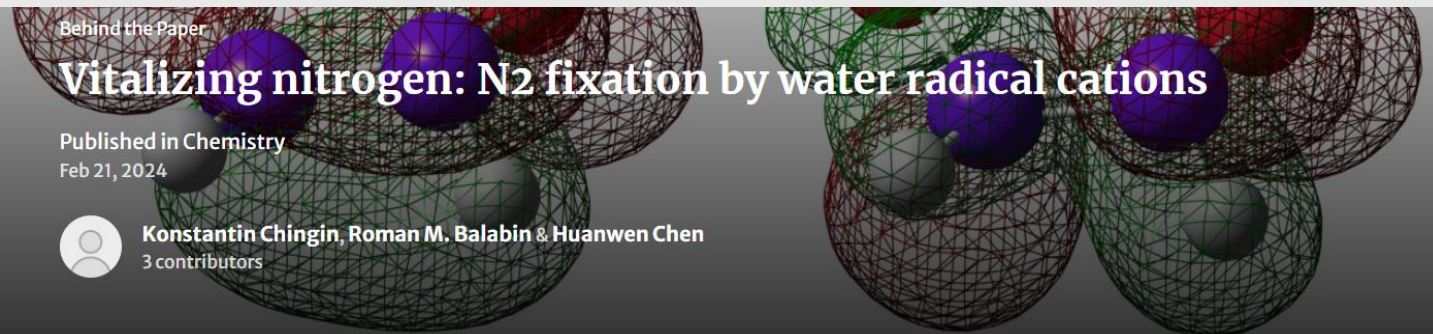


Ambient catalyst-free nitrogen fixation

- Scaled-up setup and vibrational spectroscopy:



Reaction: Press



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Жигулёвец стал соавтором нового метода связывания азота

22 февраля 2024 09:40 328

Открыт новый плазменный метод связывания атмосферного азота водой. Среди авторов – два россиянина, один из которых родился в Жигулёвске.

ПРОБЛЕМЫ И МЕТОДЫ НАУКИ

Как вода связала азот



НОВОСТИ НАУКИ

Биодоступный азот можно получить связыванием в водной плазме

18.03.2024 • РОМАН БАЛАБИН • ХИМИЯ • 68 КОММЕНТАРИЕВ



N+1

| 15:42 | 27.02.24 | * 51

| Химия

[Ссылка](#)

Молекулярный азот прореагировал с водяной плазмой
При этом образовались гидроксилламин и нитроксил

[Михаил Бойм](#)

Part V. Project Timeline

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	The reactor test & optimization	Benchmarking of recent DFT methods: SCAN, B05, and B13+ functionals	Acquiring third-party funds
	Q4			Industrial project detailing: Process engineering for nitrogen fixation by water plasma

Thank you for your attention!

感谢您的关注!

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- S8 (bottom), Lumex, PD textlogo: <https://www.lumexinstruments.com/>
- S9 (pccg), Suhm, PD textlogo: https://commons.wikimedia.org/wiki/File:GRK_782_PCGG_-_logo.gif
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