# Multiphase Chemistry & Open Access at the Interface of Earth & Life Science

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Copernicus Medal Lecture, 16 April 2015

# Acknowledgements

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**Multiphase Chemistry:** **MPIC Team & Partners**

*P. Crutzen, M. Andreae, J. Abbatt, M. Ammann, D. Knopf, T. Koop, S. Martin, E. Mikhailov, M. Molina, C. Pfrang, Y. Rudich, M. Weller, D. Worsnop, Y. F. Cheng, J. Fröhlich, C. Kampf, G. Lammel, K. Lucas, M. Shiraiwa, H. Su, B. Weber*
***& many more***

**Open Access:** **ACP Editorial Board, EGU Council & Pub. Comm., Copernicus Team, Family & Friends**

*P. Crutzen, A. Richter, T. Koop, K. Carslaw, R. Sander, W. Sturges, M. Weller, M. Rasmussen, N. Töpfer, K. Gänger, Andrea, Martin*
***& many more***

# Outline

## Multiphase Chemistry

- atmospheric & biological multiphase processes
- bioaerosols, clouds & precipitation
- reactive oxygen & nitrogen species
- human health & allergies in the Anthropocene

## Open Access

- motivation, achievements & perspectives

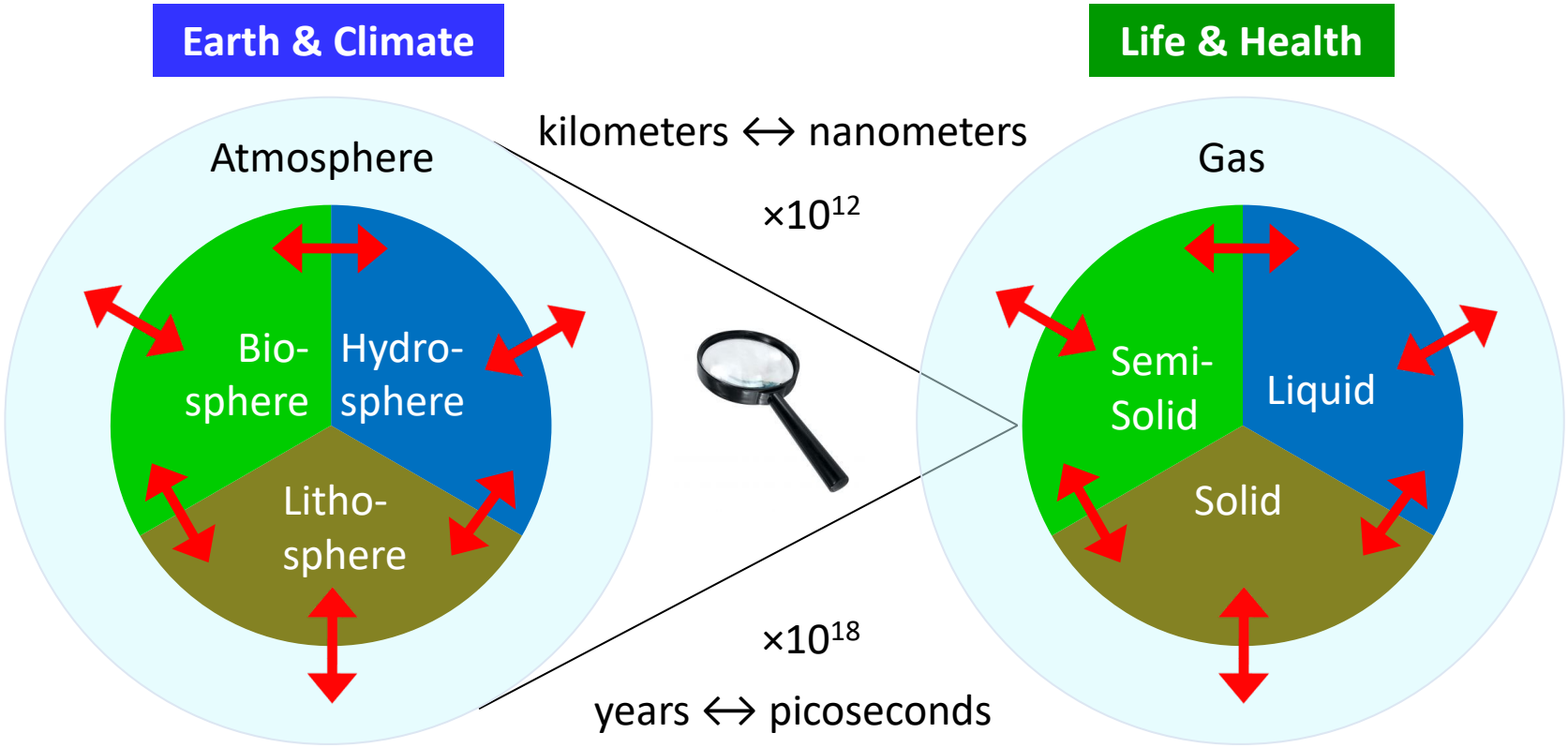
## Conclusions & Outlook

- scientific research & communication

# Multiphase Chemistry

**Interaction & transformation of gases, liquids & solids:**

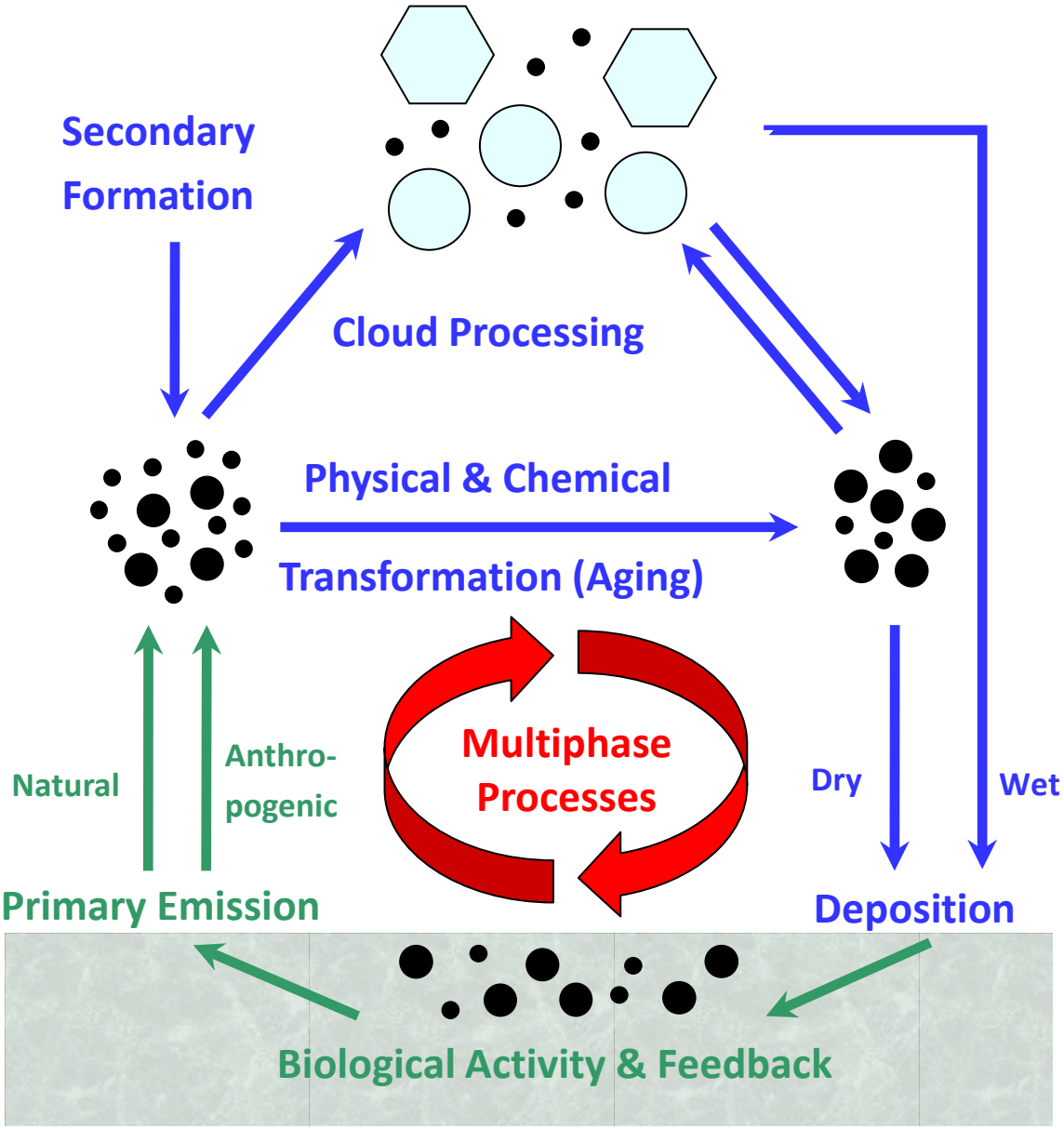
chemical reactions, mass transport & phase transitions




**Central Question:** **How does multiphase chemistry influence the Earth system & human life,** especially in the interplay of atmosphere, biosphere, climate, immune system & public health?

*Pöschl & Shiraiwa Chem Rev 2015*

# Atmosphere-Biosphere Exchange




## Atmosphere & Climate

- aerosols & gases
- clouds & precipitation
- radiation & dynamics

***Mechanistic understanding, quantitative prediction & human influence ?***

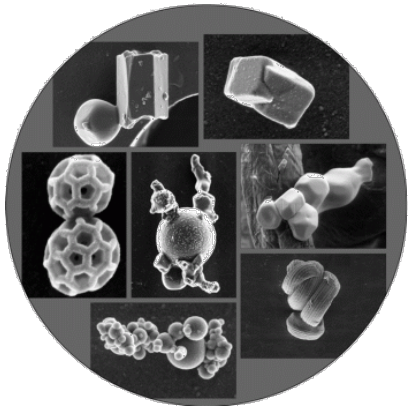
- spread & change of organisms & ecosystems
- human, animal & plant diseases

## Biosphere & Public Health

*Pöschl & Shiraiwa Chem Rev 2015*

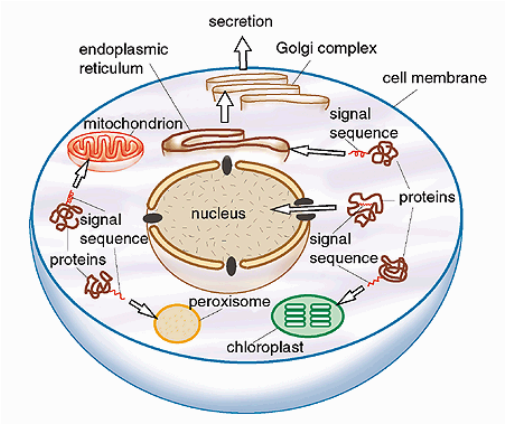
# Atmospheric & Biological Particles

**Aerosols**: solid & liquid nano- & micro-particles



**Clouds, Fog & Precipitation**: dilute aqueous particles

**Cells & Organelles**: semi-solid & liquid nano- & micro-particles




**Clouds & Fog**

**Aerosol**

**Precipitation**
(Rain, Snow, Graupel, Hail)

Gas Molecules | **Proteins** | **Viruses** | **Bacteria** | **Spores** | **Pollen** | **Uni- & Multicellular Organisms**

Sulfate, SOA, Soot

Mineral Dust, Sea Spray

**Diameter (m)**

| 1.E-10 | 1.E-09 | 1.E-08 | 1.E-07 | 1.E-06 | 1.E-05 | 1.E-04 | 1.E-03 | 1.E-02 | 1.E-01 |
|---|---|---|---|---|---|---|---|---|---|
| 100 pm | **1 nm** | 10 nm | 100 nm | **1 μm** | 10 μm | **100 μm** | 1 mm | 1 cm | 10 cm |

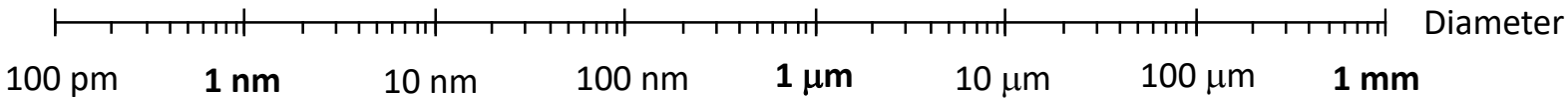
*- ultrafine -* *- fine -* *- coarse -*

*Pöschl & Shiraiwa Chem Rev 2015*

# Atmospheric & Biological Processes

**Atmosphere:** formation & interaction of gases, aerosols, clouds & precipitation

**Biosphere:** metabolism & signaling of cells & organisms

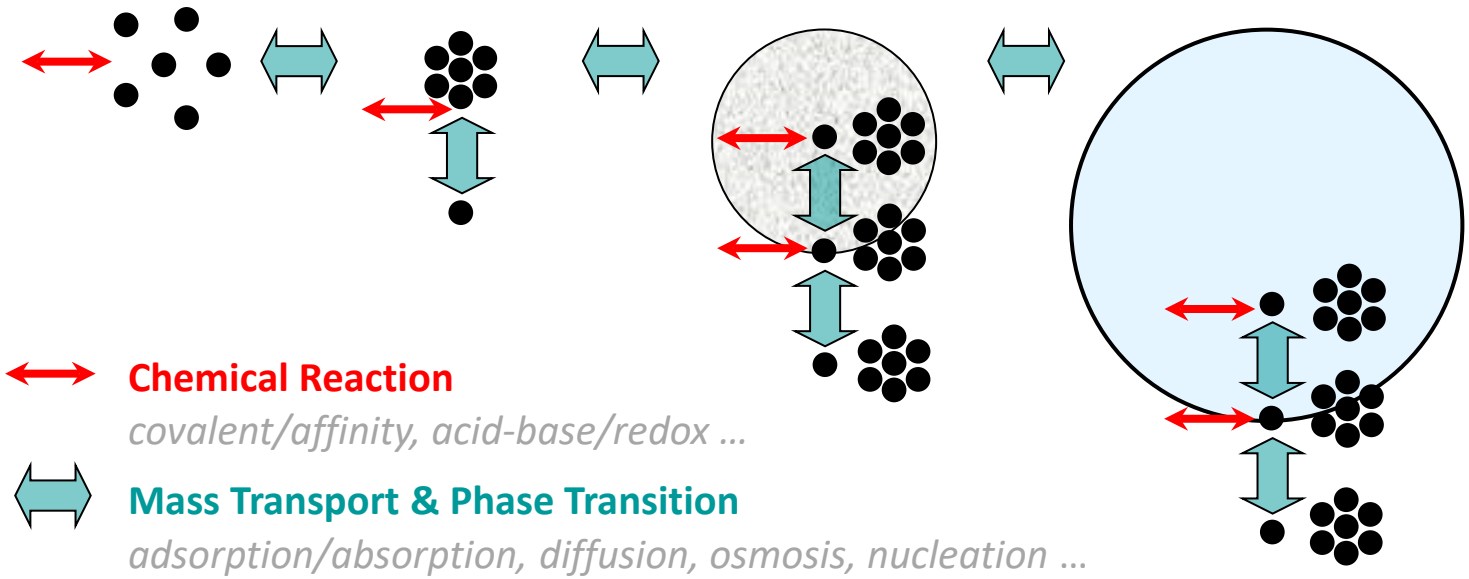



Gas Molecules
Aqueous Matrix

Molecular Clusters
Biopolymers

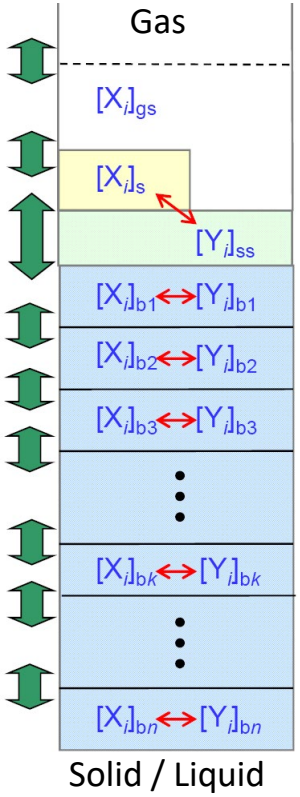
Aerosol Particles
Membranes, Organelles

Clouds & Precipitation
Cells, Organisms



**Chemical Reaction**
*covalent/affinity, acid-base/redox …*

**Mass Transport & Phase Transition**
*adsorption/absorption, diffusion, osmosis, nucleation …*




**Common Denominator:** analytical techniques, chemical kinetics & molecular dynamics, kinetic & thermodynamic models (KM-GAP …)

*Pöschl & Shiraiwa Chem Rev 2015*

# Multiphase Chemistry Department @ MPIC Mainz

**Earth Science**

**Aerosols & Regional Air Quality**
***Y. Cheng*** *et al.*
*Minerva Group*

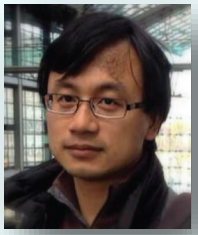
regional & global cycling

**Semivolatile Organic Compounds**
***G. Lammel*** *et al.*

**clouds, precipitation,** nanoparticles

gas-particle partitioning

**Aerosol, Cloud & Biosphere Interactions**
***H. Su*** *et al.*



**Organic Aerosols & Oxidants**
***M. Shiraiwa*** *et al.*

**reactive nitrogen, surface exchange**

reaction kinetics & mechanisms, **reactive oxygen species & radicals**

**Multiscale Interactions & Integration**
***U. Pöschl*** *et al.*

**Cryptogamic Covers**
***B. Weber*** *et al.*
*Crutzen Stipend*

**microorganisms,** biodiversity ice nuclei

**proteins, allergens,** pathogens

**Inflammatory Processes**
***K. Lucas*** *et al.*

**Life Science**

**Bioaerosols & Microbiology**
***J. Fröhlich*** *et al.*

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- **bioaerosols, clouds & precipitation**
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## Conclusions & Outlook

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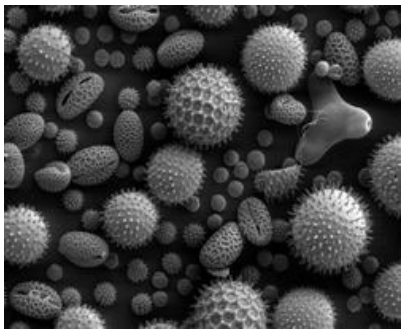
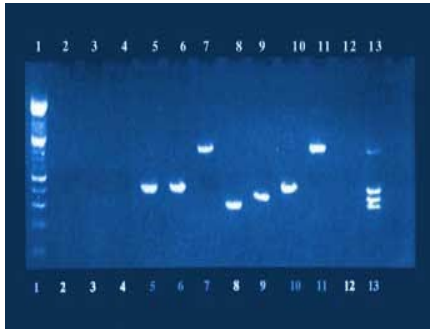
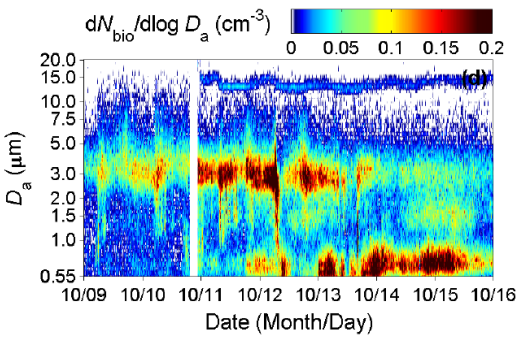
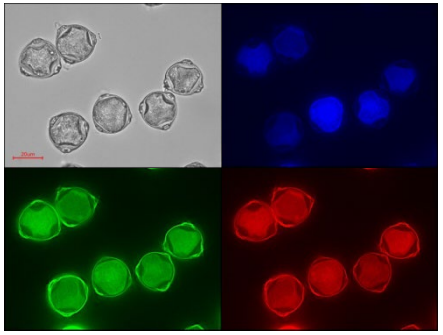
# Bioaerosols






DNA & Protein Analysis



Fluorescence Spectroscopy & Microscopy

**High abundance, diversity & fluxes of airborne bacteria & fungi**

~1 µg $m^{-3}$, ~10 $L^{-1}$, **~$10^2$ $m^{-2}$ $s^{-1}$**, >$10^3$ species (urban PM)

**"Life is in the Air":** ~10 ng $m^{-3}$ DNA

⇒ inhalation of ~1 µg/day ≡

**~$10^6$ bacterial genomes/day**

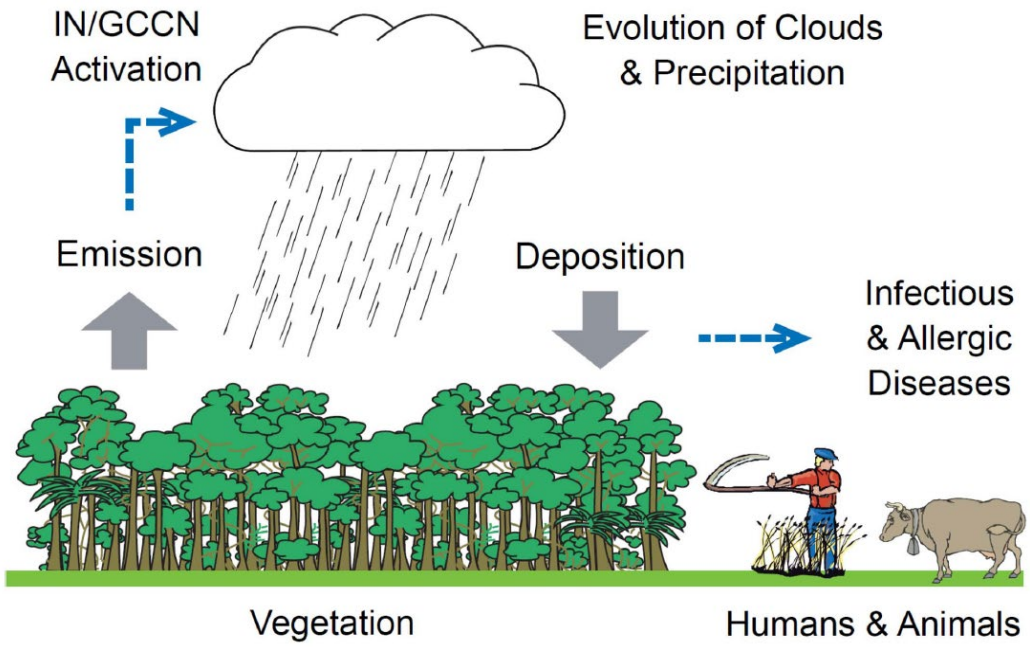
**Pathogens:** permanent challenge

**⇒ infectious & allergic diseases**

**Cloud condensation & ice nuclei:**

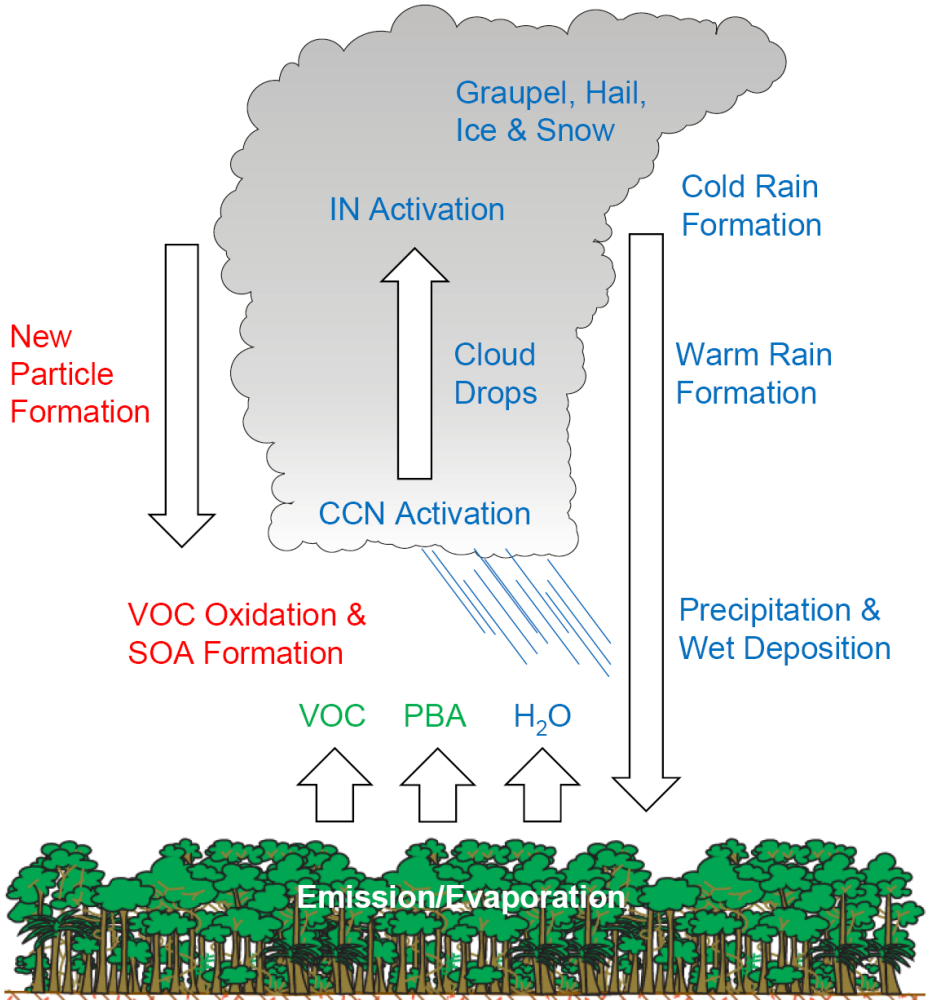
co-evolution of life & climate

**⇒ bioprecipitation cycle**



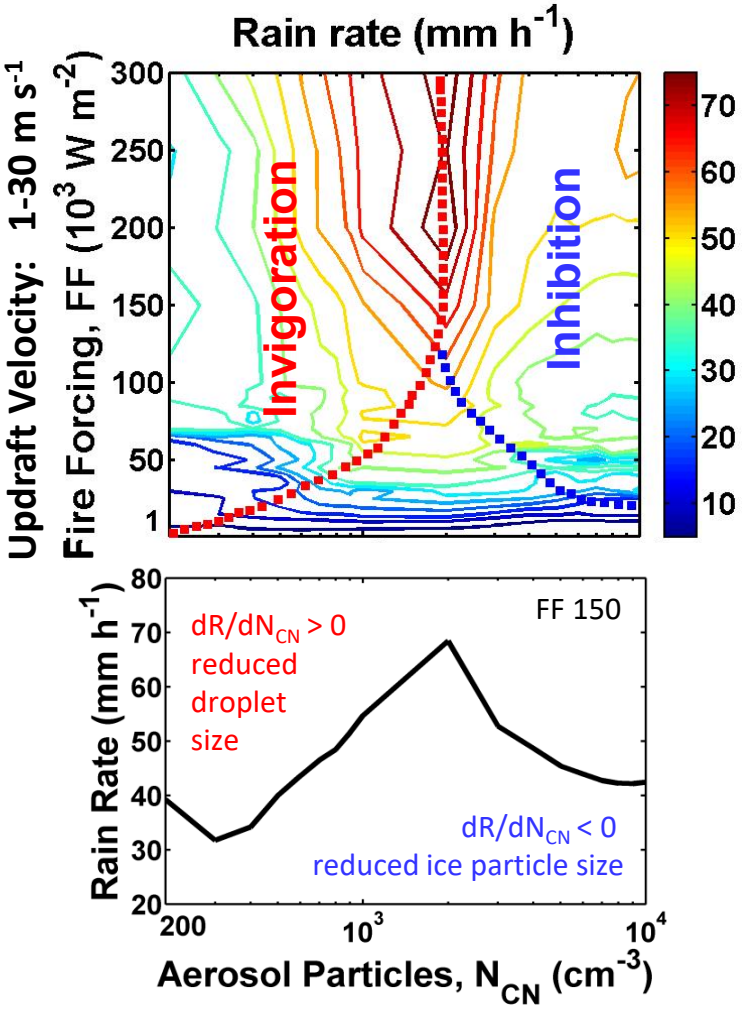

*Elbert et al. ACP 2007, Fröhlich et al. PNAS 2009, BG 2012, 2014, Despres et al. Tellus 2012 Pöhlker et al. AMT 2012, 2013, Science 2012, Huffman et al. ACP 2013, Morris et al. GCB 2014*

# Aerosol-Cloud-Precipitation Interactions




**Amazon rainforest as biogeochemical reactor**
generating nuclei for clouds, ice & precipitation

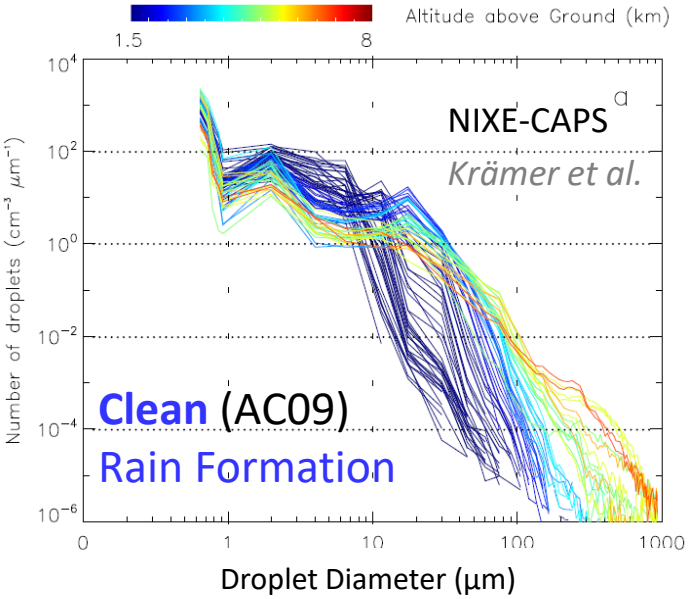
*Pöschl et al. Science 2010*

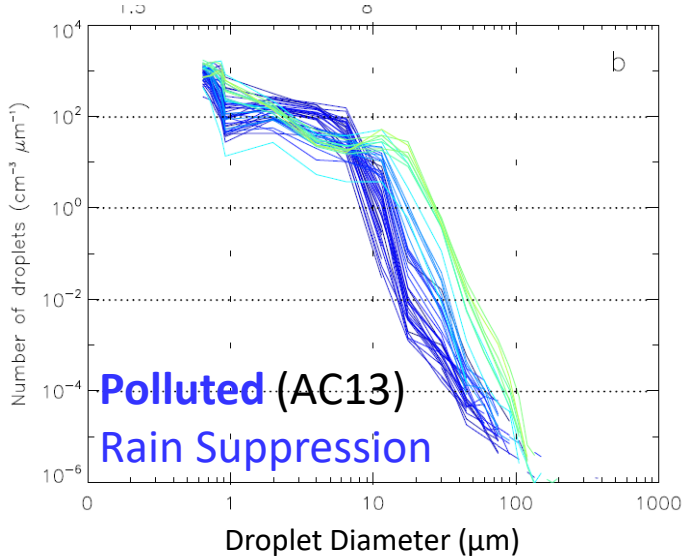



**Aerosol effects on rainfall in convective clouds**
with charact. regimes of invigoration (clean) & inhibition (polluted)

*Reutter et al. ACP 2014; Chang et al. ACPD 2014*

# Comprehensive Profiling of Aerosols, Clouds & Precipitation




**ACRDICON-CHUVA campaign:** HALO research aircraft, September 2014, collaboration with GoAmazon/IARA, large international team (Brazil, Germany, USA …)

*Wendisch et al. BAMS 2015*

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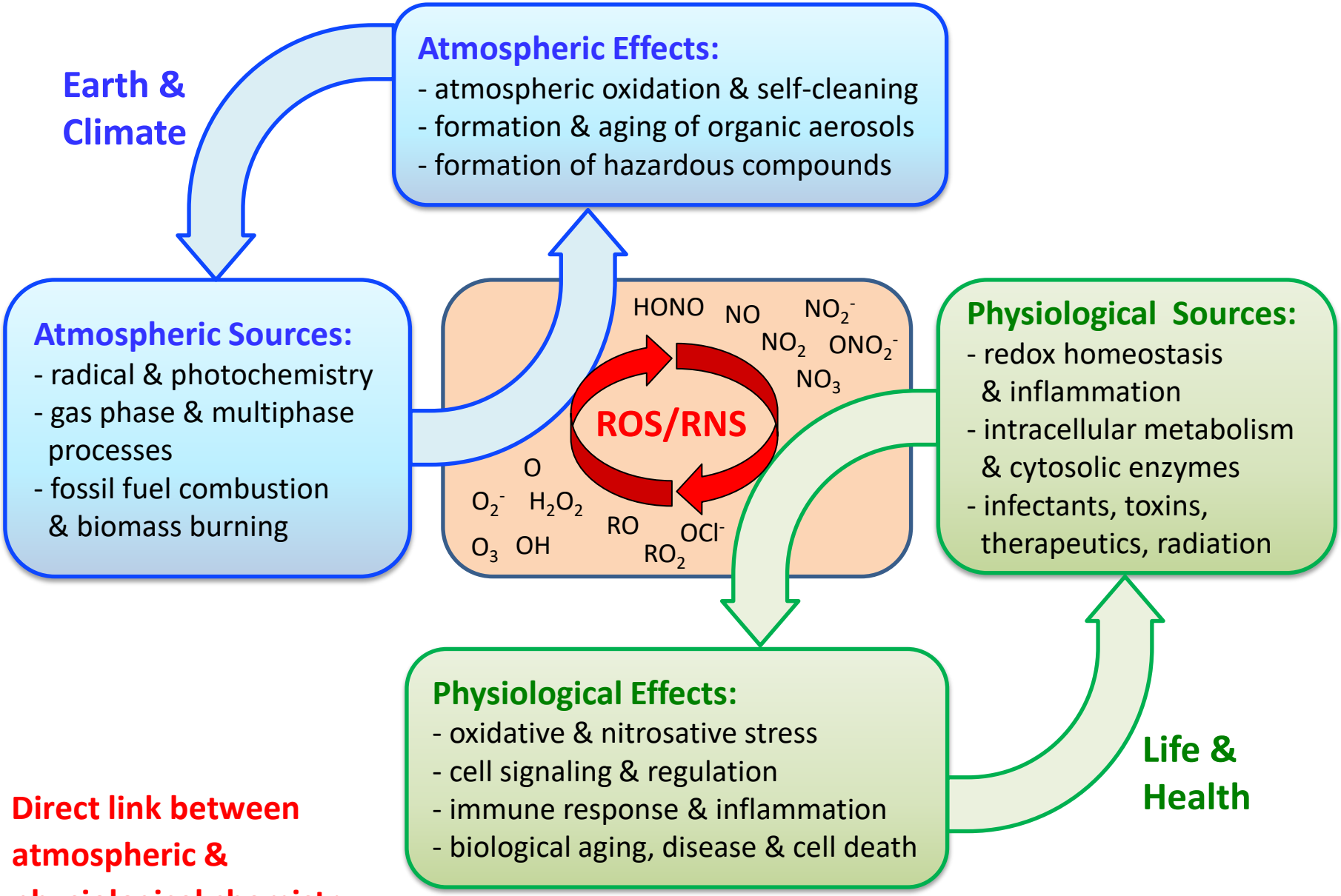
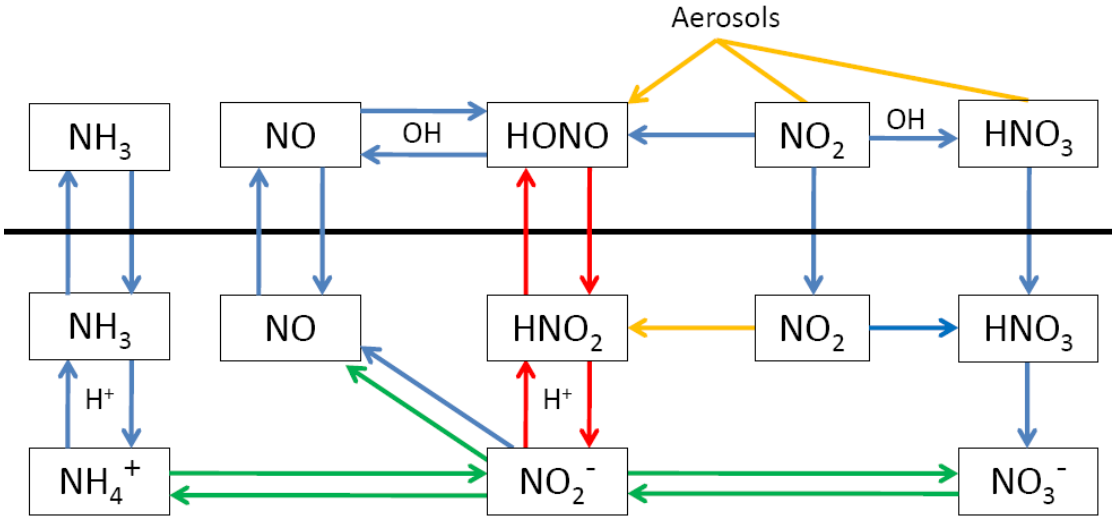
# Reactive Oxygen & Nitrogen Species




**Direct link between atmospheric & physiological chemistry**

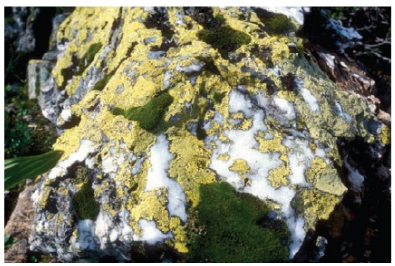
*Pöschl & Shiraiwa Chem Rev 2015*

# Nitrogen Cycling through Soil & Cryptogamic Covers

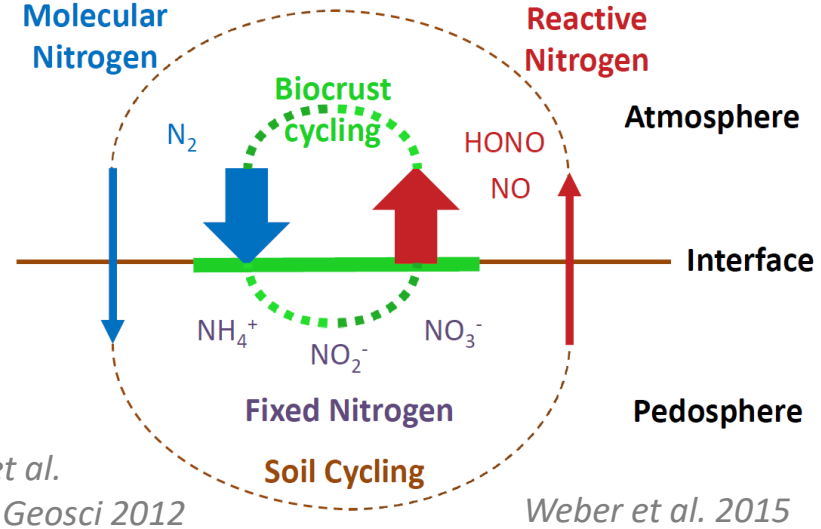



**Nitrous acid emissions from soil nitrite & microbes:**
**major source of atmospheric RNS & ROS** (OH radicals)

*Su et al. Science 2011,*
*Oswald et al. Science 2013*



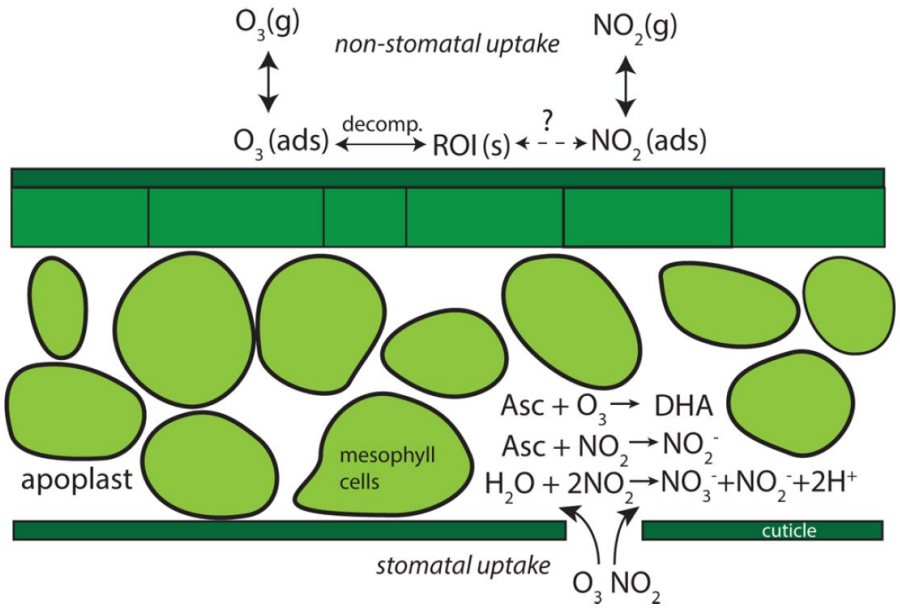

*Elbert et al.*
*Nature Geosci 2012*




*Weber et al. 2015*

**Cryptogamic covers on soil, rock & plants** (lichens, mosses, cyanobacteria …):
**major contributors to $N_2$ fixation** (up to ~50% of global terr. BNF) **& RNS emissions ?**

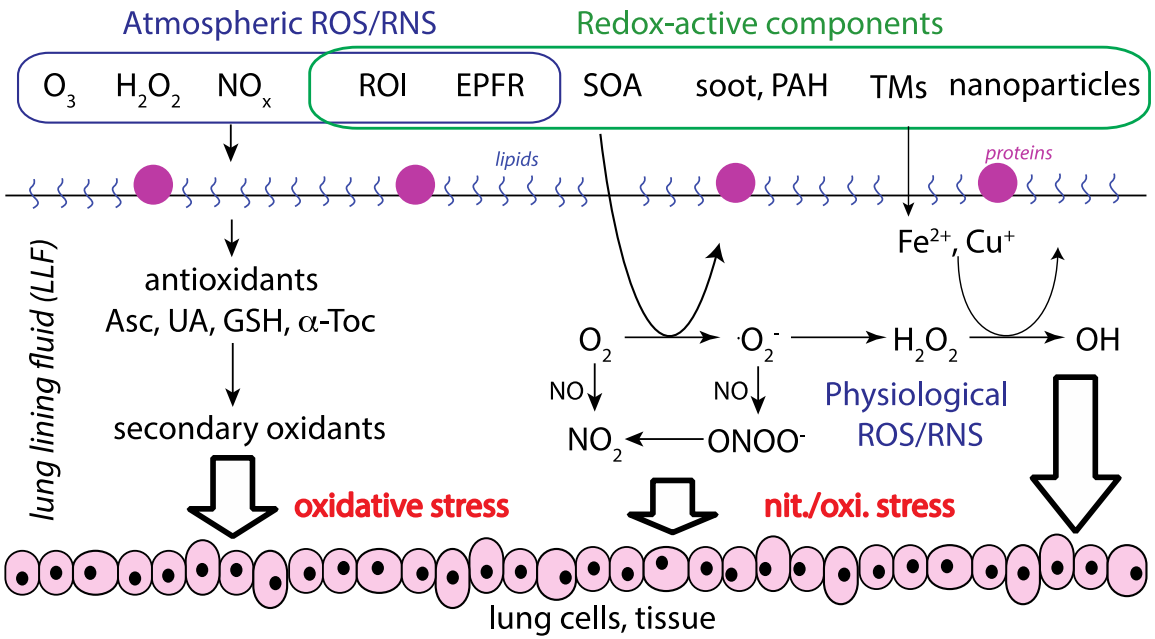
# ROS/RNS Cycling through Plant Leaves & Human Lungs




**Uptake of $O_3$ & $NO_2$ by plant leaves:**

- bulk uptake through plant stomata & reaction with ascorbic acid
- surface reaction involving reactive oxygen intermediates ?

*Pöschl & Shiraiwa Chem Rev 2015*




**Oxidative stress in human lungs:**

- inhalation of atmospheric ROS/RNS only partly buffered by antioxidants
- formation of ROS/RNS through aerosol particle reactions *(soot, metals, …)*
- quantification & health effects ?

*Pöschl & Shiraiwa Chem Rev 2015*
*Lakey et al. 2015*

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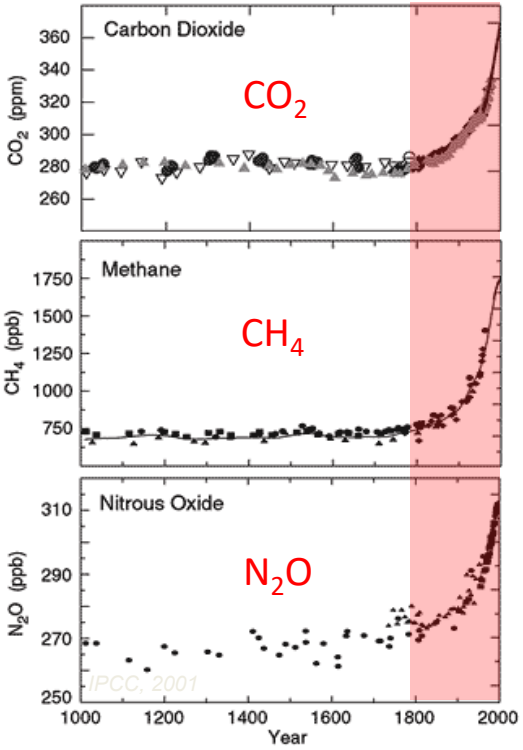
# The Anthropocene – A New Age in Earth & Human History


THE ANTHROPOCENE

*Paul Crutzen, Anthropocene Symposium, Mainz, Dec. 2013*

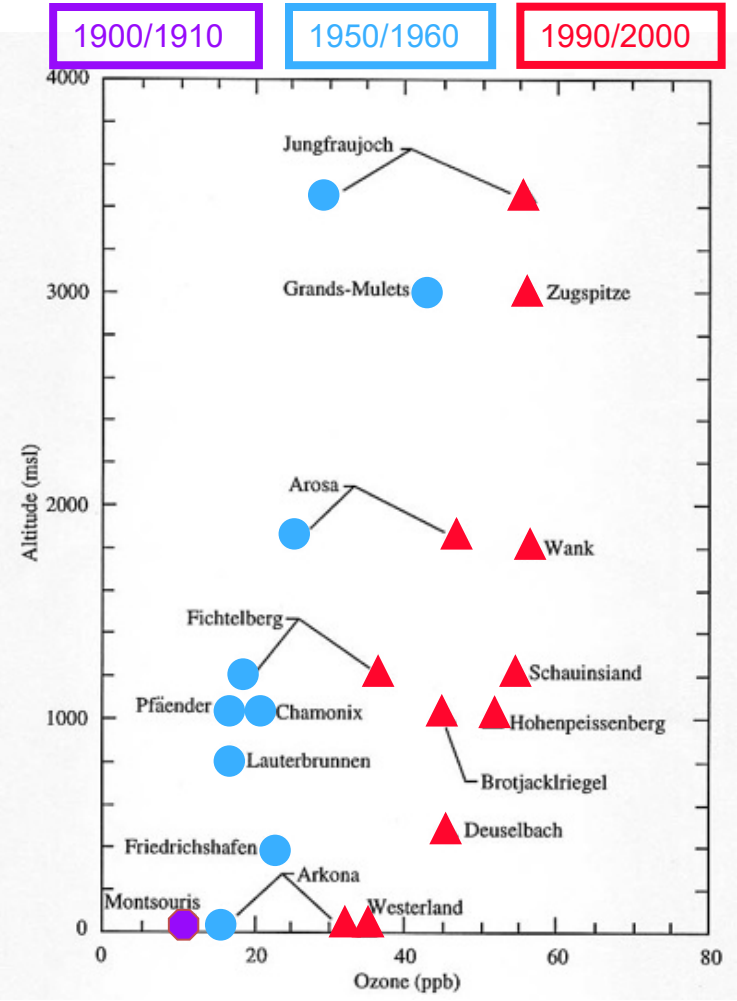
**Scientific curiosity meets practical challenges: Earth System Science & Global Change from scientific discovery to political & societal action**

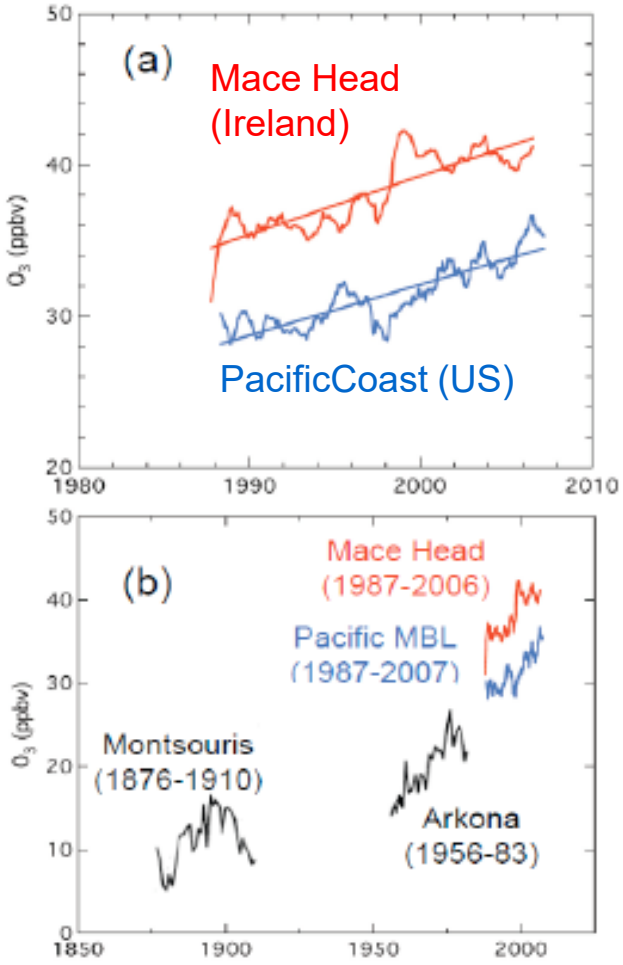
| | |
|---|---|
| **Ozone Hole & CFC:** | success story – discovery, controversy & discussion, solution |
| **Climate Change & GHG:** | political & scientific struggle – complexity & predictability |
| **Public Health & PM/ROS:** | new challenges – oxid. stress, allergy & chronic inflammation |

**Scientific & societal message: We are shaping the planet, so let‘s get it right …**

*Crutzen Nature 2002, Anthropocene Symposium Mainz 2013, Pöschl & Shiraiwa Chem Rev 2015*

# Surface Ozone & Aerosol Increase in the Anthropocene



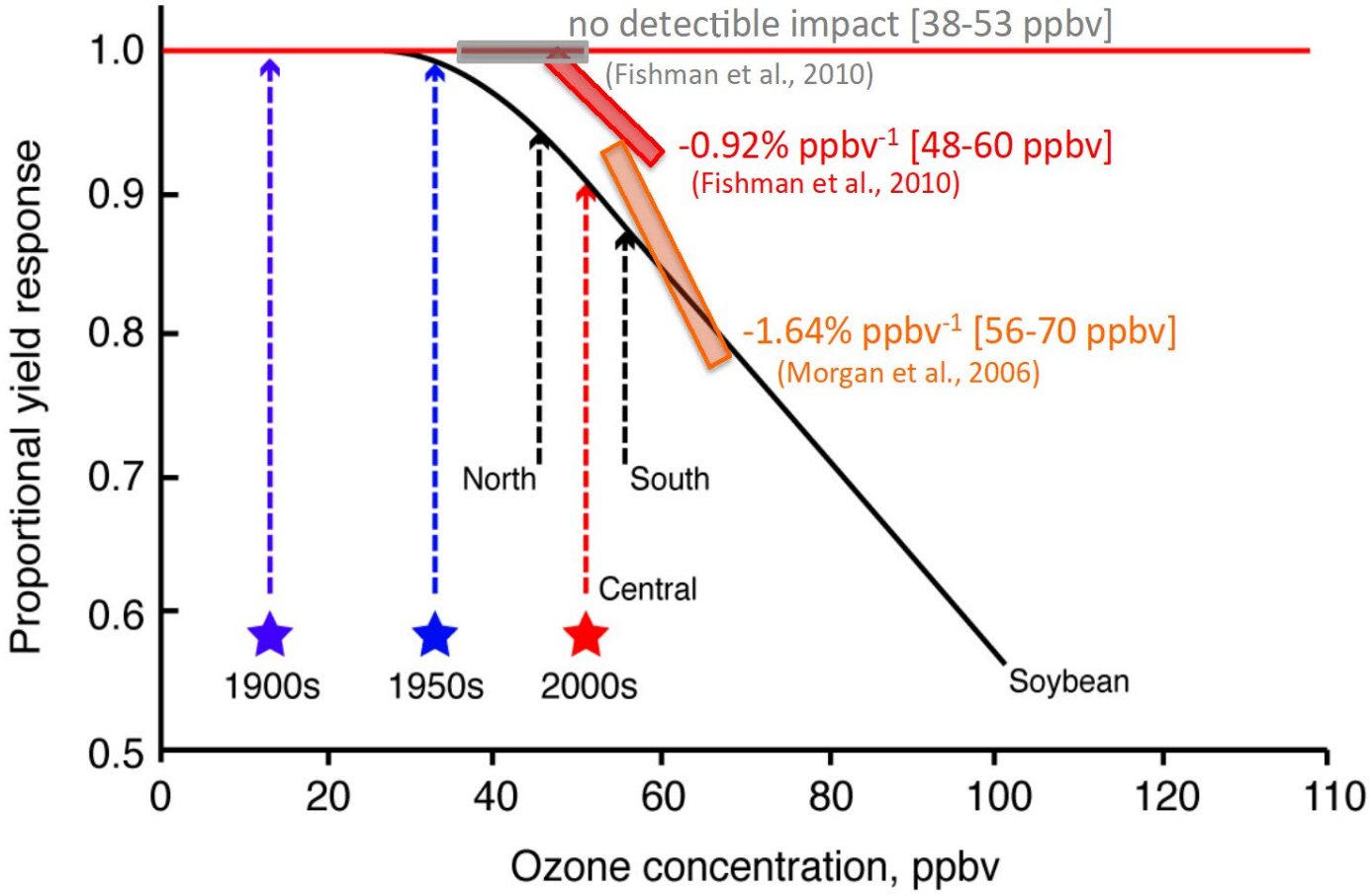

**Ozone:** **2-fold background increase** (from 10-20 ppb to 30-40 ppb)

**Aerosol:** **10-fold enhancement in polluted regions**

($10^3$–$10^5$ cm$^{-3}$ & 10–100 µg m$^{-3}$ vs. $10^2$–$10^3$ cm$^{-3}$ & ~1–10 µg m$^{-3}$)

*Staehelin AE 1994, Parrish ACP 2009, Cooper Nature 2010, Fishman 2013; Pöschl & Shiraiwa Chem Rev 2015*

# Decreasing Crop Yields due to Ozone




**Toxic ozone background concentrations** in southern USA reduce yields of various crops (soy, wheat, cotton, potato, etc.):

**Are we creating a toxic atmosphere?**

*Haegle 1989, Morgan et al. 2006, Fishman et al. 2010, Fishman 2013*

# Increasing Allergies due to Air Pollution ?

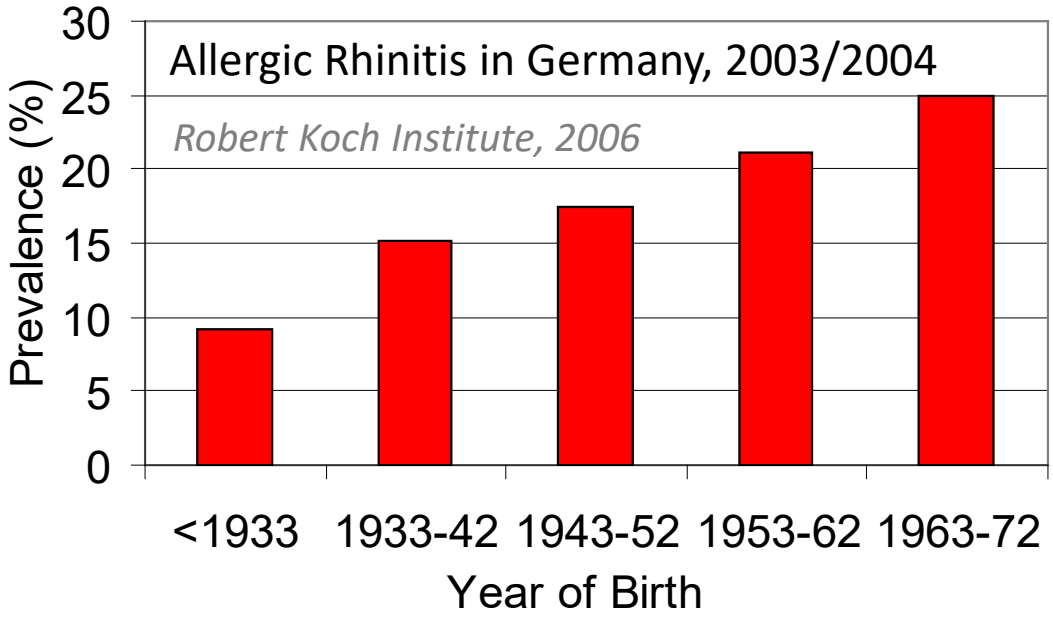
## High Prevalence

~ 30 % of population in
W. Europe & N. America
affected by allergic diseases
*(rhinitis, asthma, dermatitis;*
*food allergies, etc.)*

## Steep Increase

~ 3 % per decade over past 50 years

⇒ *50% prevalence by 2050,*
*"epidemic of 21st century" ?*




## Negative Social & Economic Effects

impairment of personal well-being & workforce productivity, health care expenses, etc.

⇒ *estimated macroeconomic costs: 25 billion EUR/yr for EU (similar for US)*

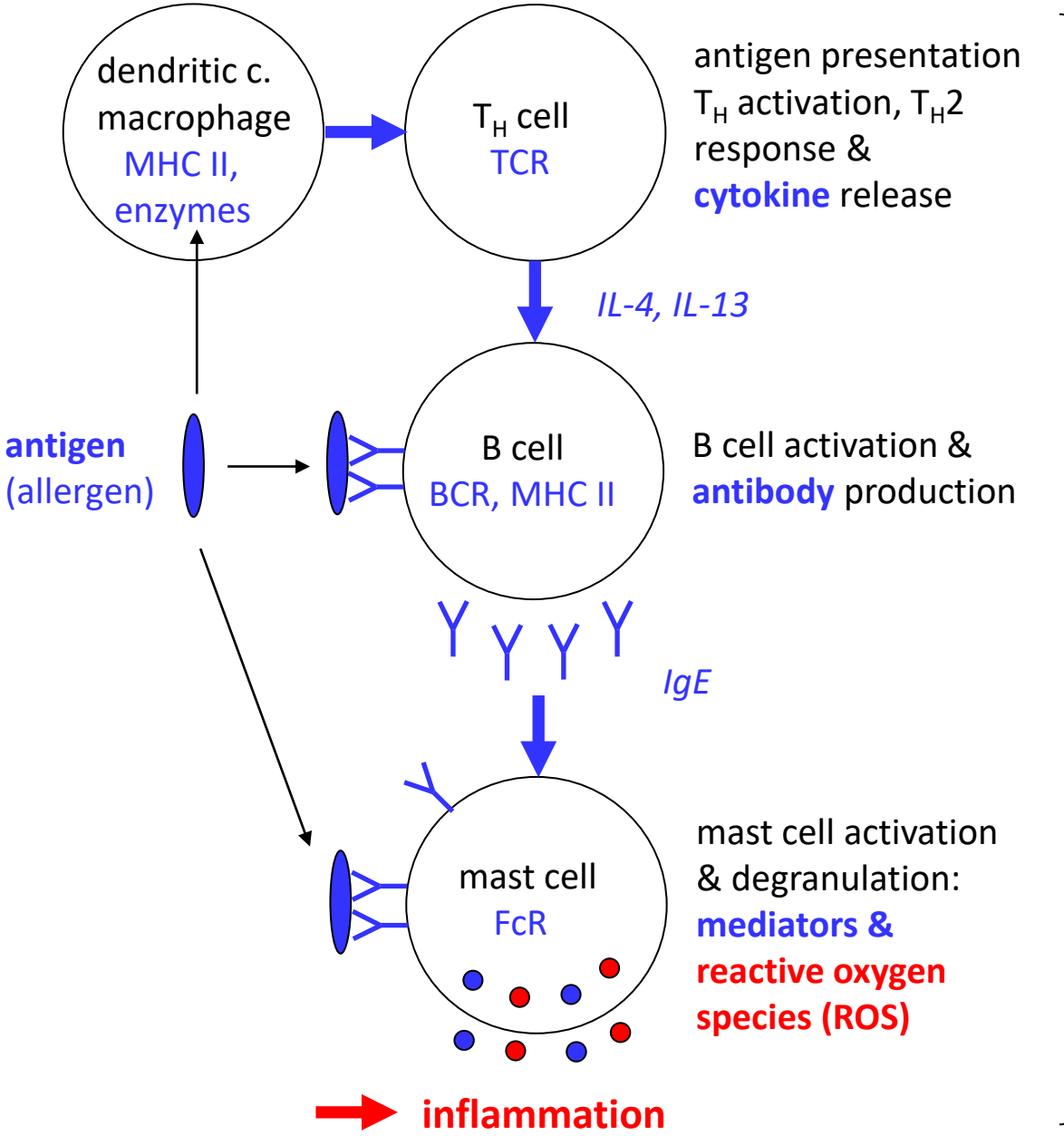
## Correlation with Urbanization & "Western Lifestyle"

trends in E. Europe, Asia & developing countries similar to W. Europe & N. America

⇒ ***no solid explanation, just hypotheses: hygiene, nutrition, stress, pollution***

⇒ ***chemical mechanism of air pollutant effects?***

# Allergic Reaction = Protein Multiphase Chemistry

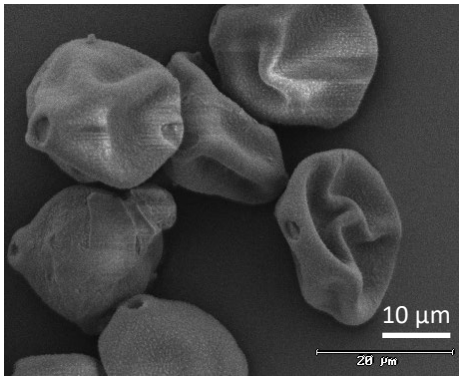


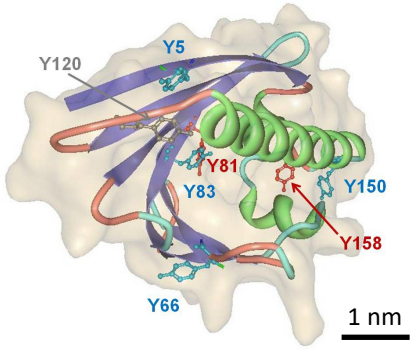

**Regulation & signaling of immune system = multiphase chemistry of protein molecules** in liquids & semi-solids

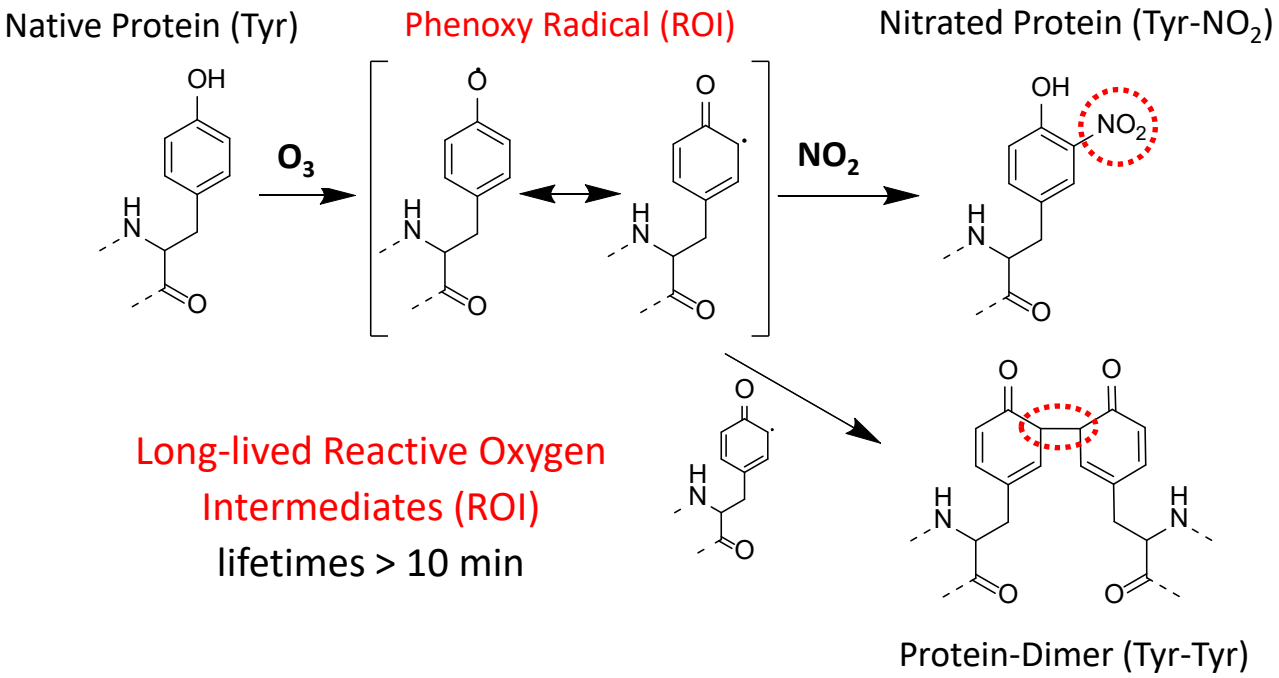
**Chemical modification** can influence each step of **protein interaction** (affinity binding)

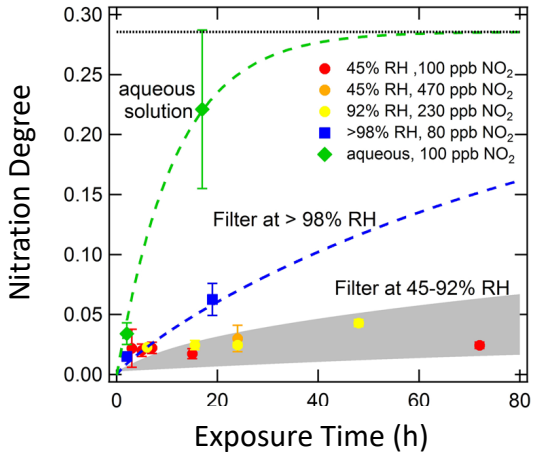
Normal function of IgE & inflammation: **parasite defense**
**allergy = false alarm**

# Protein Nitration & Oligomerization




**Birch pollen allergen Bet-v-1 exposed to $O_3$ + $NO_2$**

⇒ enhanced allergenicity of nitrated & oligomerized products

⇒ **mechanistic rationale for promotion of allergies by large-scale air pollution in the Anthropocene**

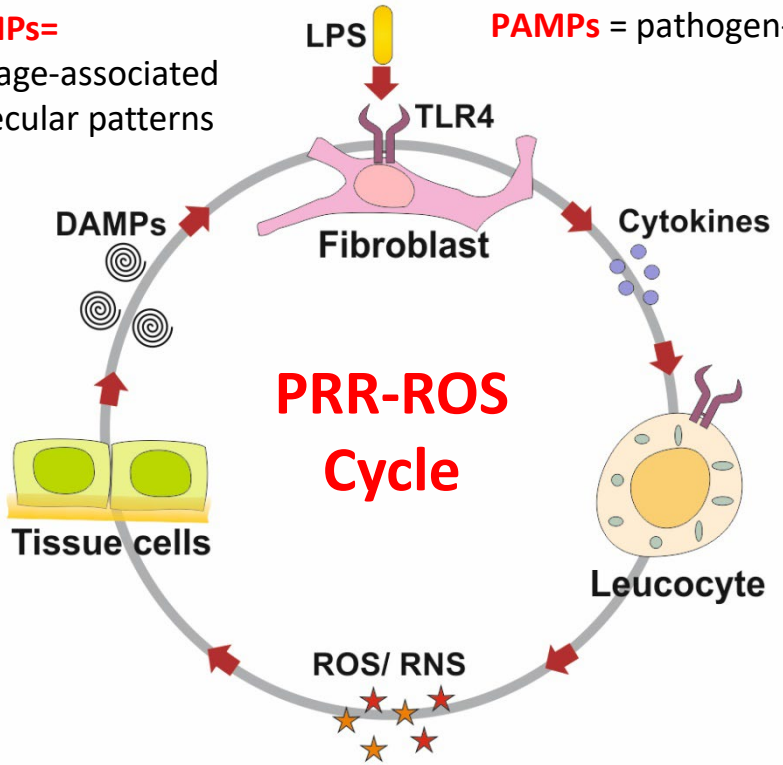
⇒ **concentration thresholds for adverse health effects & chemical reaction pathways of immune response ?**

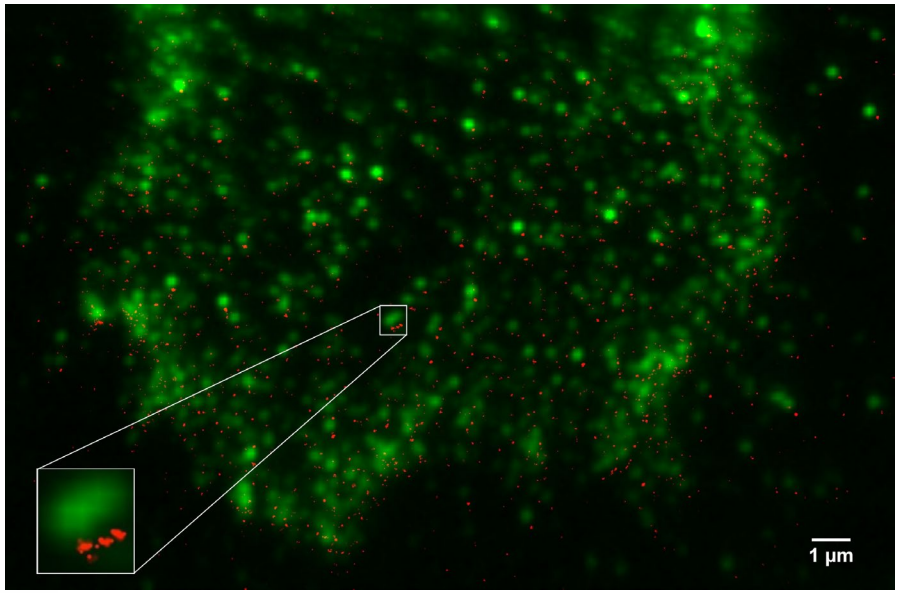
*Franze et al. EST 2005, Gruijthuijsen et al. IAAI 2006, Shiraiwa et al. Nature Chem 2011, EST 2012, Reinmuth-Selzle J Proteome Res 2014, 2015*

# Chemical Pathways of Human Immune Response

**DAMPs=** damage-associated molecular patterns

**PAMPs** = pathogen-associated molecular patterns, e.g., LPS = lipopolysaccharide




Fluorescence detection of toll-like receptors (TLR/PRR)

**Chemical amplification & feedback through pattern recognition receptors (PRR)**

⇒ **allergies & chronic inflammation**

**Quantify & simulate** reaction kinetics & amplification factors (KM-SUB-PRR)

**Localize** reaction sites by immunostaining & superresolution microscopy (~10-100 nm)

*IMB Mainz, U Heidelberg, C. Cremer et al.*

**Interrupt** cycle by receptor blocking (herbal extracts) & ROS quenching (molec. hydrogen)

⇒ ***Mainz Center for Chemical Allergology***, *JGU Translational Immunology, D. Schuppan et al.*

*Lucas Mol Neurobiol 2013, Lucas et al. 2015*

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# Motivation for Open Access

***Scientific, educational & economic advantages of free online availability & usability of** (publicly funded) **research publications.***

## Educational:

- inform & stimulate interested public *(school teachers, students, et al.)*
- equal opportunities in the information society *(global & social)*
- re-integrate scholarly & common knowledge *(wikipedia, etc.)*

## Economic & Technological:

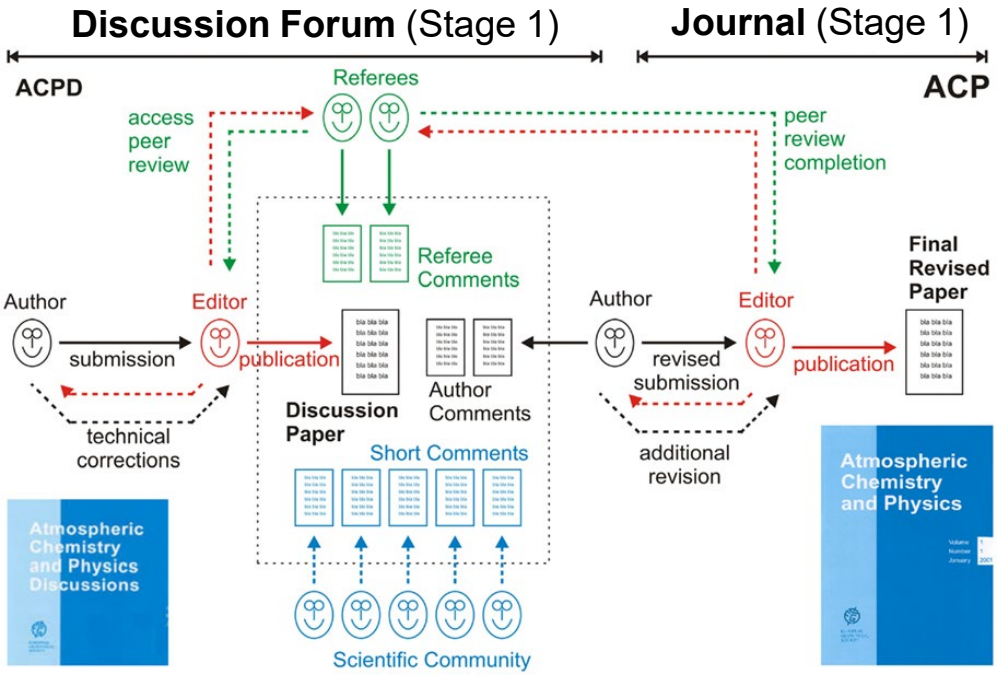
- liberate distorted scientific information market *(prod., distrib., copyright, archiving)*
- facilitate technological applications & innovations *(text mining by SME, etc.)*

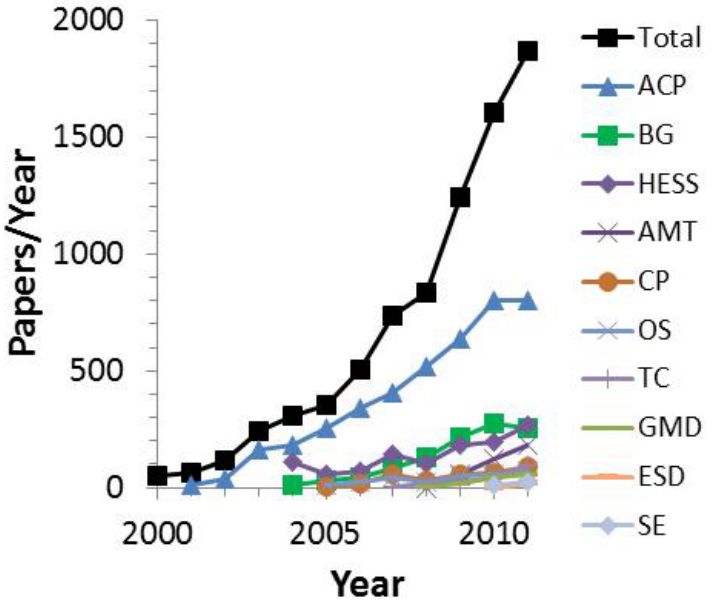
## Scientific:

- enhance interdisciplinary exchange *(access & usage)*
- foster discussion & peer review *(public commenting, etc.)*
- advance evaluation & quality assurance *(machine-reading & statistics, transparency & new metrics beyond citation counting oligopoly)*

*Pöschl, Frontiers Comput. Neurscience 2012*

# Interactive OA Publishing & Public Peer Review




Combine strengths of traditional peer review with virtues of transparency & self-regulation

Key features: free speech & high speed; public scrutiny & interactive discussion

⇒ save refereeing capacities; maximize quality assurance & information density

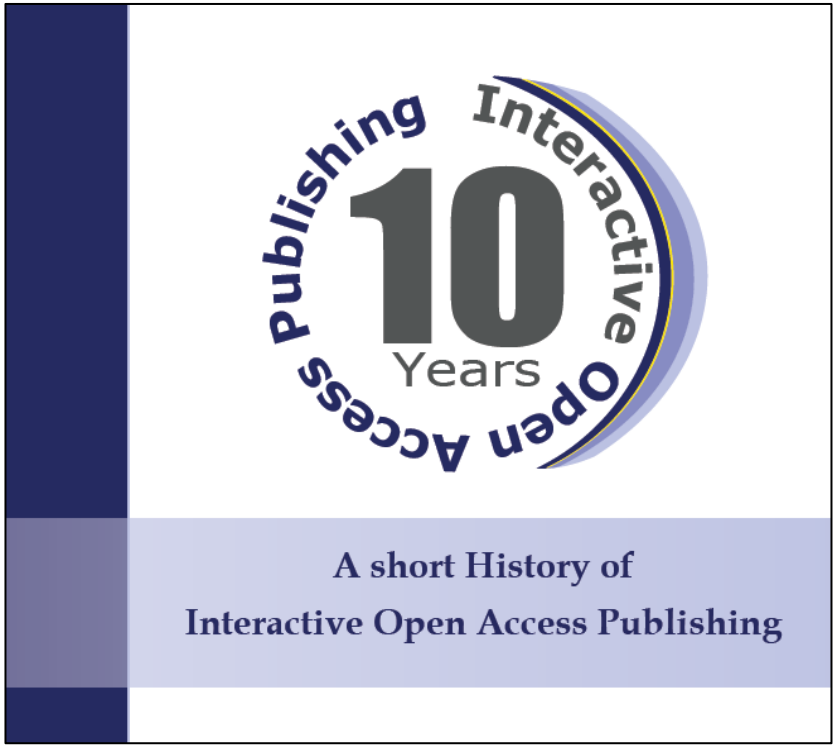
⇒ document open questions, controversial opinions & scientific discourse

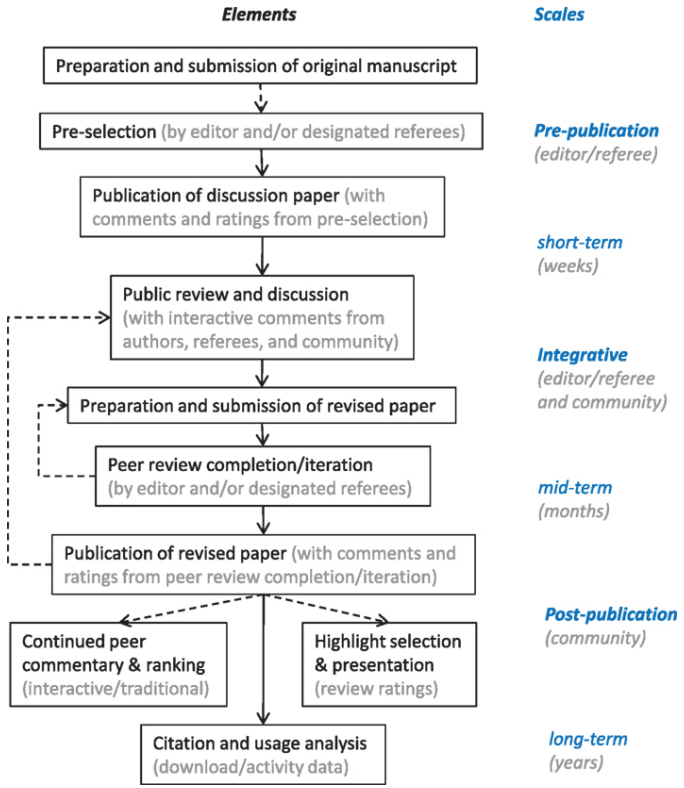
Unique combination of achievements:

top speed, top impact & visibility, large volume, low rejection rates

*Pöschl, Frontiers Comput. Neurscience 2012*

# Past Developments & Future Perspectives




**Short history booklet:** origins & background of an amazing journey *(Paul Crutzen)*
*http://www.copernicus.org/A_short_History_of_Interactive_Open_Access_Publishing.pdf*

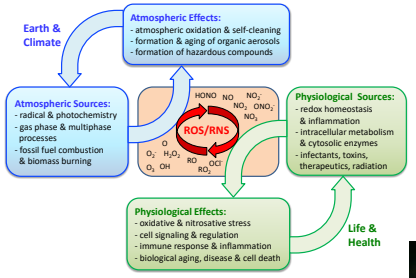
**Multi-stage open peer review article:** repositories *(arXiv.org)*, rankings & usage statistics …
*http://journal.frontiersin.org/article/10.3389/fncom.2012.00033/abstract*

**Vision:** **promote scientific & societal progress through global information commons**
⇒ **epistemic web** *(along & beyond web 2.0/3.0, semantic web …)*

# Conclusions & Outlook

**Interdisciplinarity in Earth & Life Science:**

The grass is always greener under the fence;
lots of exciting research & discoveries ahead.



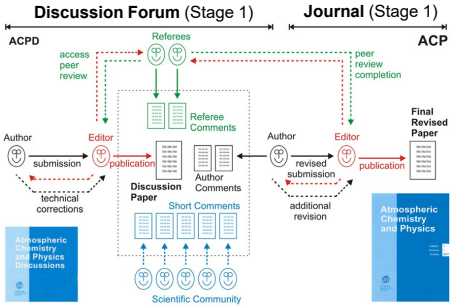

**Climate & Health in the Anthropocene:**

We are shaping the planet, so let‘s get it right.

*- with special thanks to Paul Crutzen*


**Open Access & Public Peer Review:**

Let‘s share more & better information
for the benefit of science & society.




**Innovation:**

Think big, go for it & do it yourself.

*- with special thanks to Arne Richter*