Cross-Scale Water Dynamics to Mechanistically Inform Plant Phenotyping and Productivity Models

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EASTERN REGIONAL PHOTOSYNTHESIS CONFERENCE

UNIVERSITY OF WYOMING

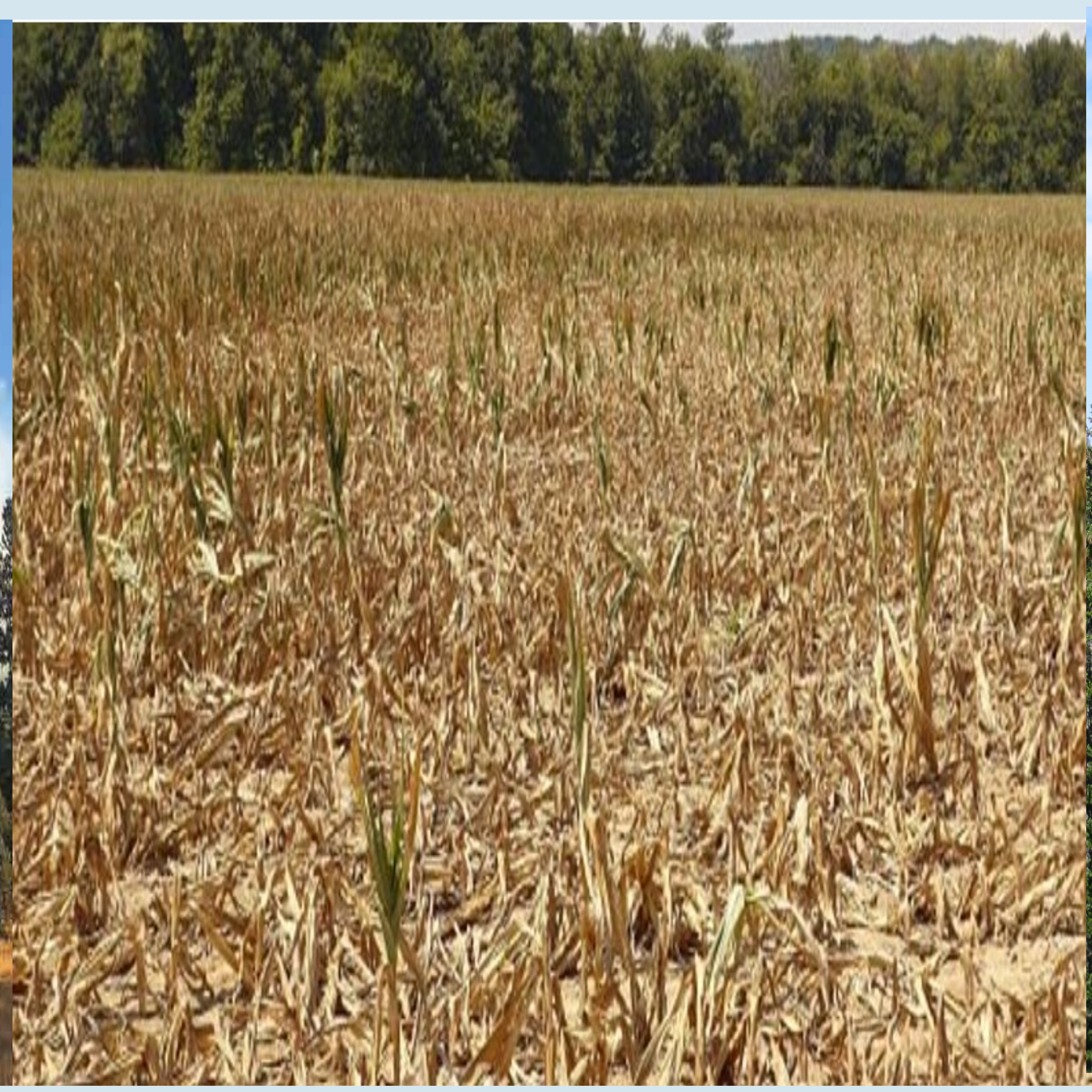
Current Headaches for Plant Scientists:

- **How can we improve predictions of plant productivity and plant stress response under a changing environment?**

- **How can we breed and select for novel genotypes better fit for unknown future environments?**

- **Improve photosynthesis (Simply A MUST!)**





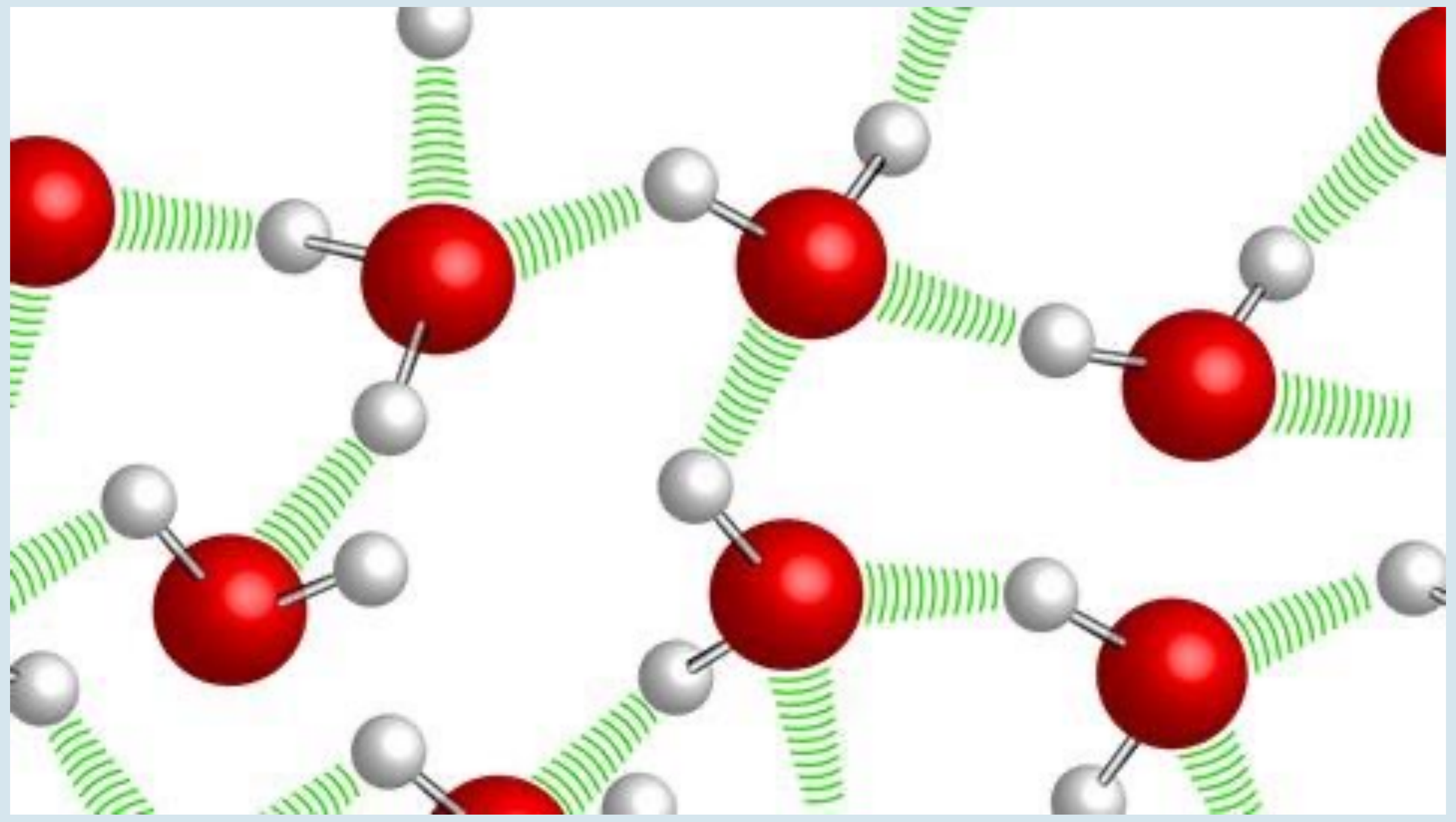

The Question:

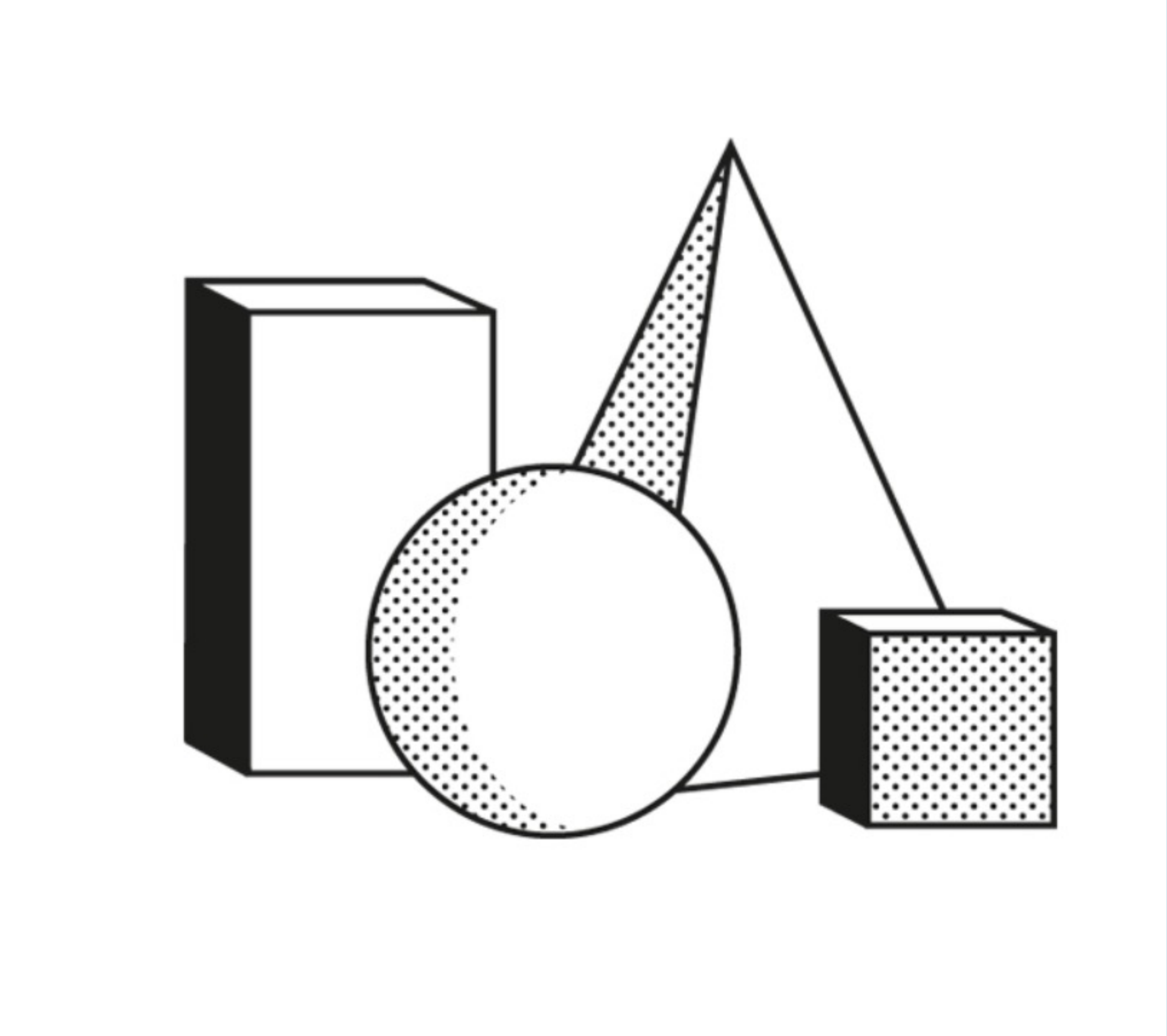
What are the characteristics of a good **predictive trait ?**

- Scalability (dynamics follows time & space)
- Applicability (can be used on diverse species and genotypes - discriminates stress phenotypes)
- Robust high-throughput
- <u>Be able to provide mechanistic information – **Informed Phenotyping**</u>

Mechanistic Information Provided by Biophysical Processes

- These include mass and energy budgets and all subatomic, atomic, or molecular process in an organism that involves passive, physical movement; attraction or repulsion (electrostatic, van der Waals, gradient, hydrogen bonding, hydrophobic, hydrophilic, etc.)

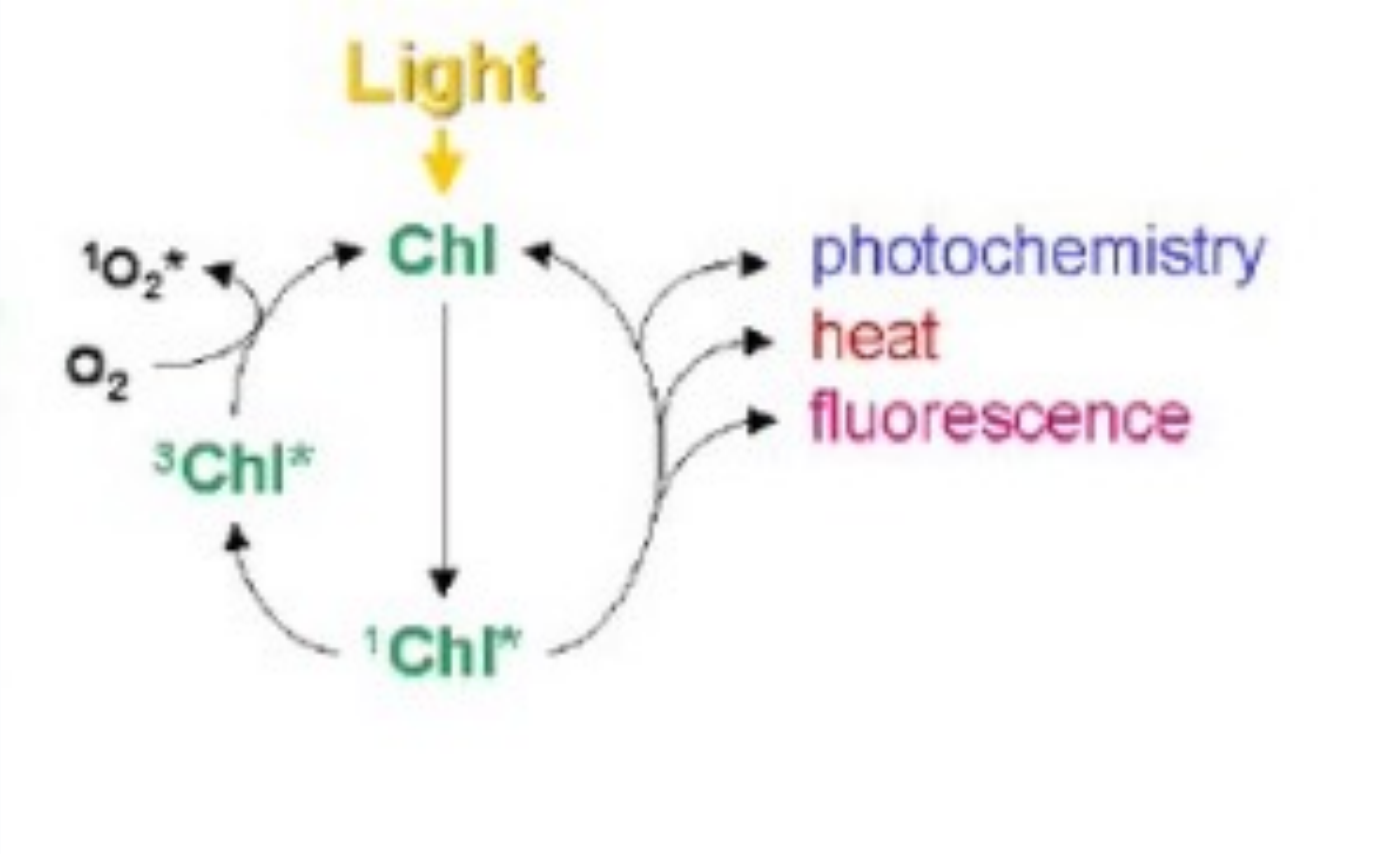


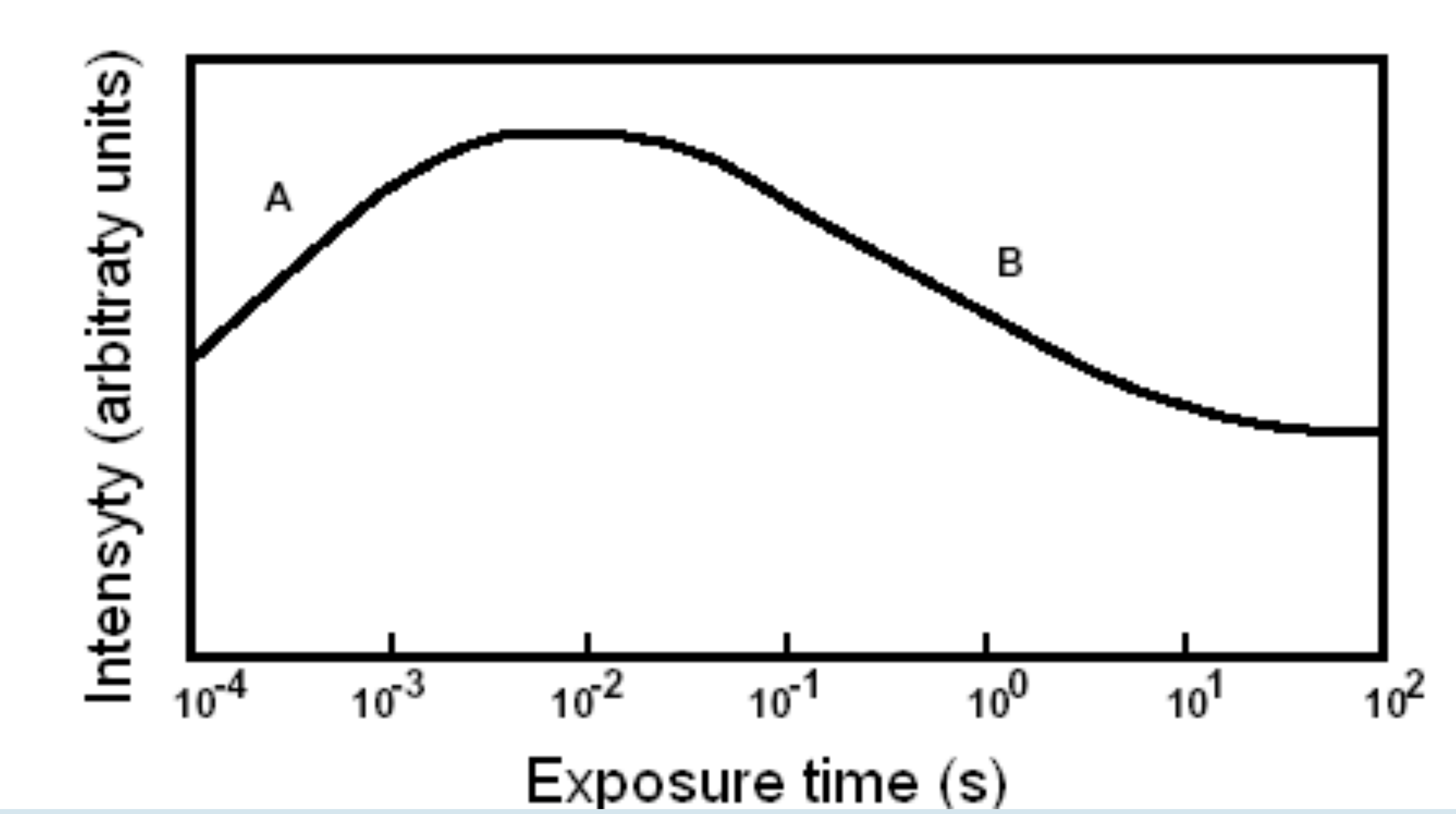


- ➢ The integration of biophysically relevant traits that can be dissected to **first principles** (i.e., the building blocks of complex systems based on fundamental physical theories) is critical to implemented and informed predictions

Chlorophyll a Fluorescence:

- Informative of photochemical and non-photochemical processes
- Non-invasive
- Scalable
- Widely applicable – from cyanobacteria to green algae and all plants
- Fast
- High-throughput and currently widely used means of PSII efficiency





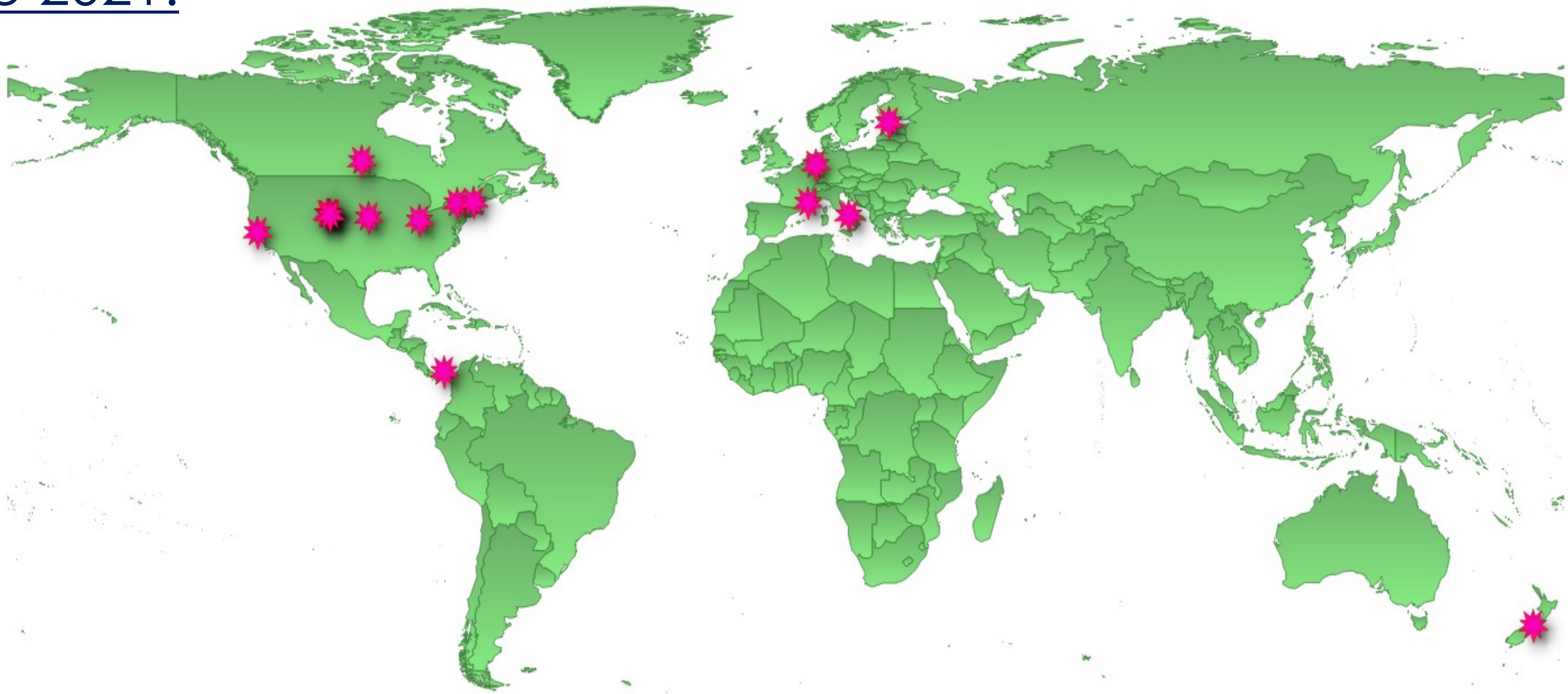
Kautsky H., Hirsch A. (1931). "Neue Versuche zur Kohlensäureassimilation". Naturwissenschaften. 19 (48): 964. Bibcode:1931NW.....19..964K. doi:10.1007/bf01516164.

Chlorophyll a Fluorescence:

*Shabala S.N. (**2002**) Screening plants for environmental fitness: chlorophyll fluorescence as a ‘**Holy Grail’ for plant breeders**. In Advances in Plant Physiology, Vol. 5. (ed. A. Hemantaranjan), pp. 287–340. Scientific Publishers, Jodhpur, India.*

In 20 years have we made significant progress?

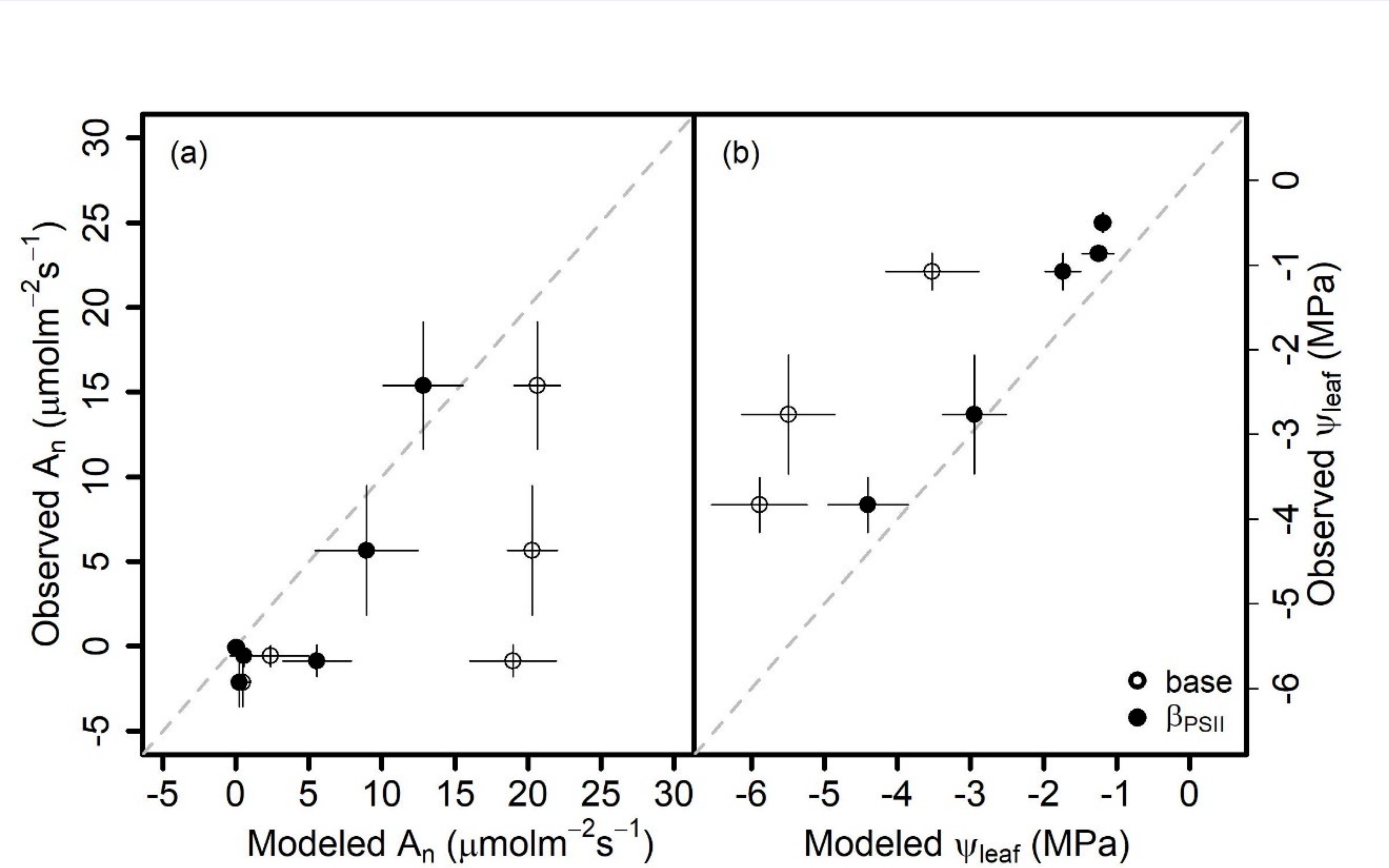
Chlorophyll *a* Fluorescence Network – updated to 2021:



B. E. Ewers, C. Weinig (UW); D. Beverly (Indiana University); M. Bretfeld (Kennesaw University); S. D. McKay, J. Pleban, D. Kim (SUNY), C.R. McClung (Dartmouth College), K. Greenham (University of Minnesota), T. Awada, A. Tasos, V. Stroeger, T. Pabst (UNL), Y. Yarkhunova (M. Planck, Cologne, Germany), M. Salmela (Luke, Helsinki, Finland), R. Baker (Miami University), N. D'Ambrosio (Federico II, Naples, Italy), K. Niyogi (UC, Berkeley), M. Kessler (ETH, Zurich, Switzerland)

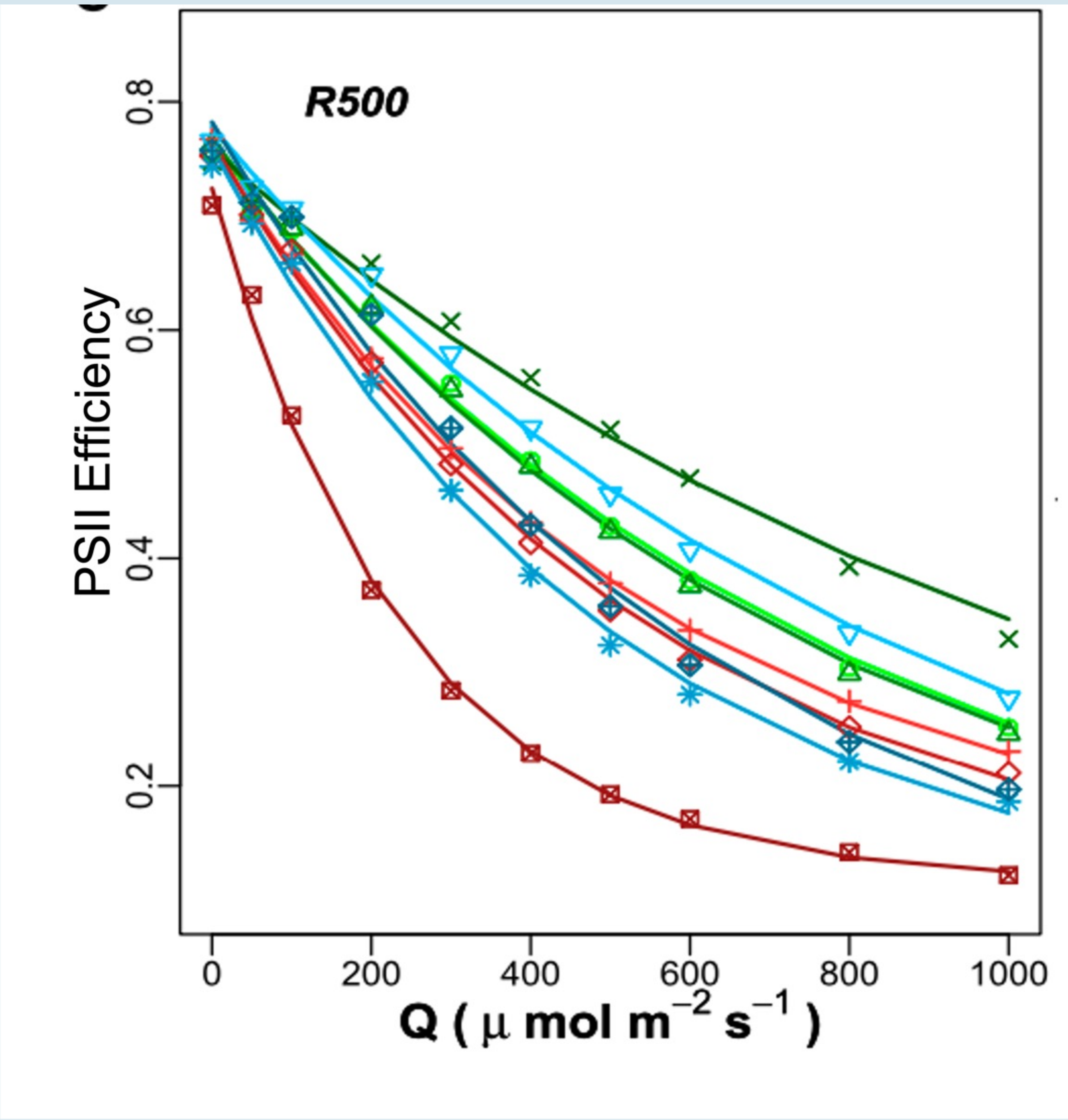
Improved productivity modeling:

- Chl *a* Fluorescence variables and biophysical parameters improve whole plant productivity predictions (TREES model) and existing photosynthesis models (FvCB model)



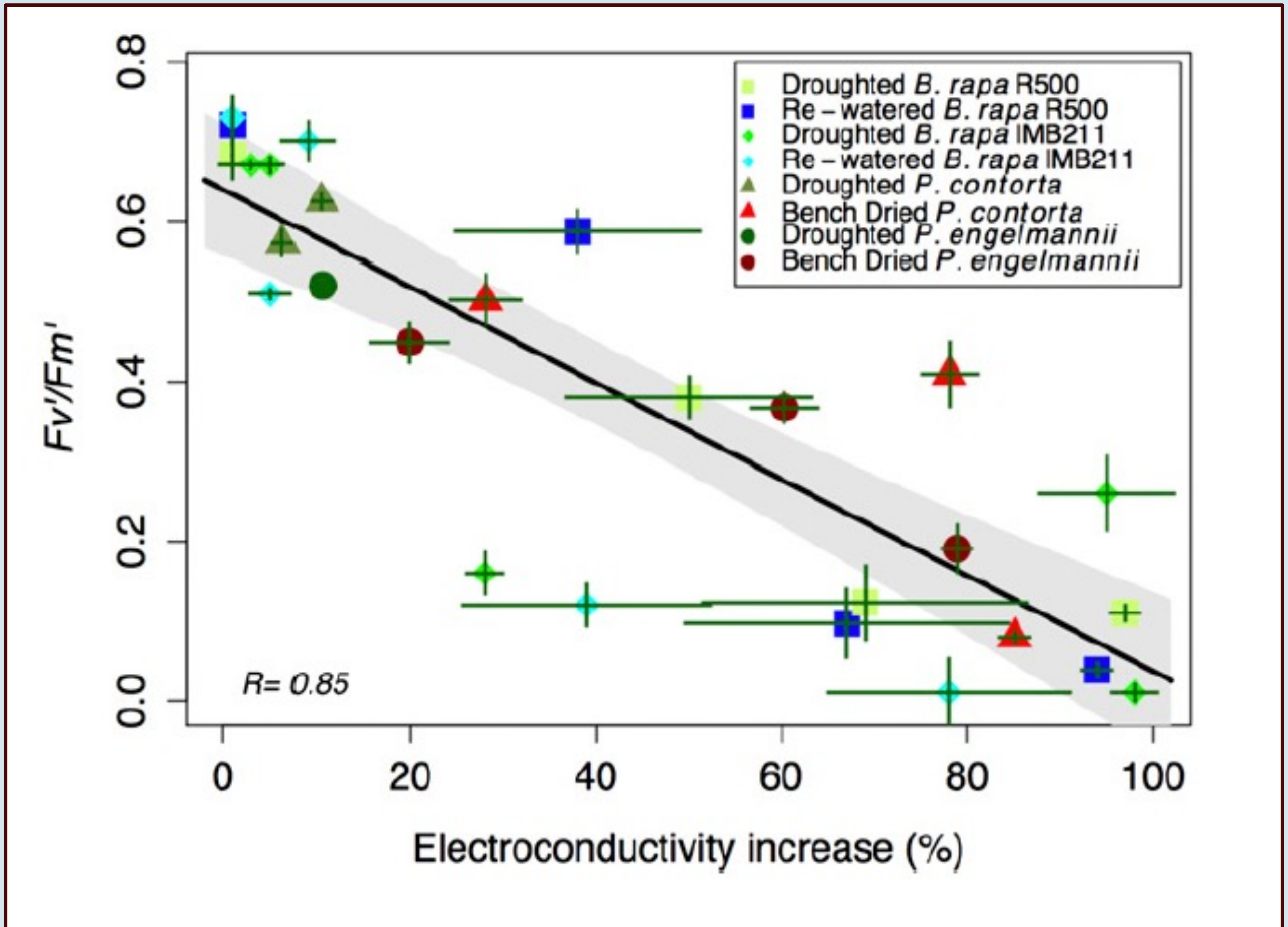
Kim*, Guadagno *et al.* –
Plant Cell & Environment, under review

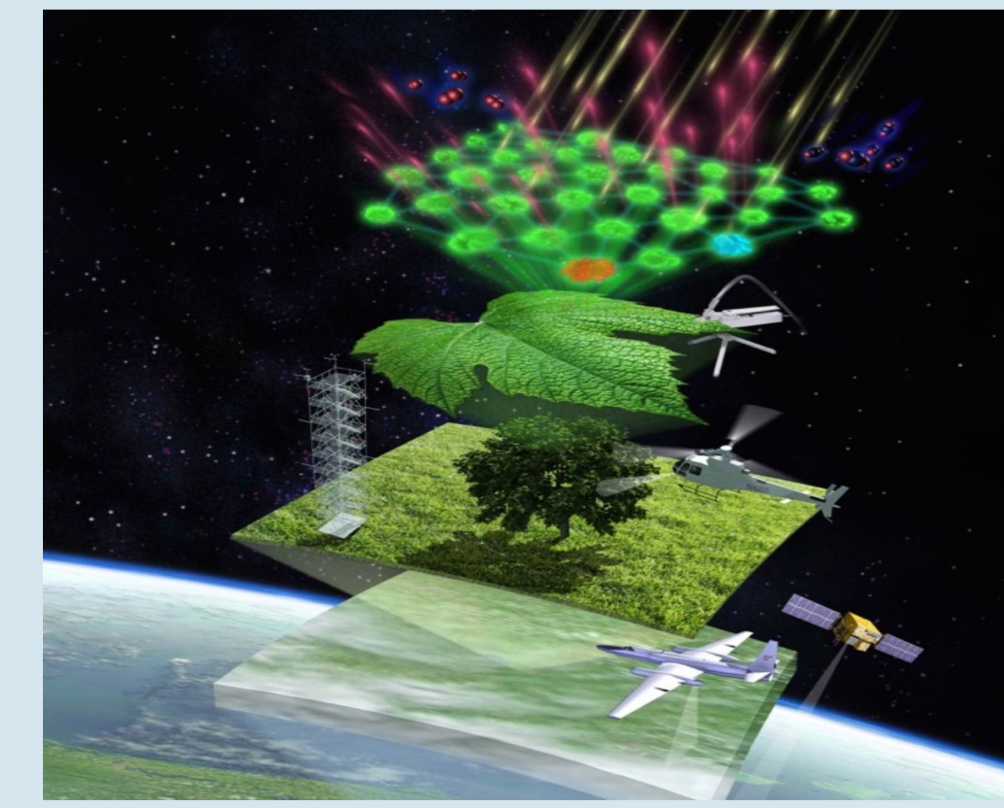
Pleban*, Guadagno* *et al.* –
Plant Physiology, 2020



Chl a Fluorescence recovery & mortality:

- Chl *a* Fluorescence variables and biophysical parameters represent robust cross-species means of death by drought – What does the water do?





Guadagno *et al.* – Plant Physiology, 2017

Water availability has shaped photosynthetic evolution and adaptation around the globe:

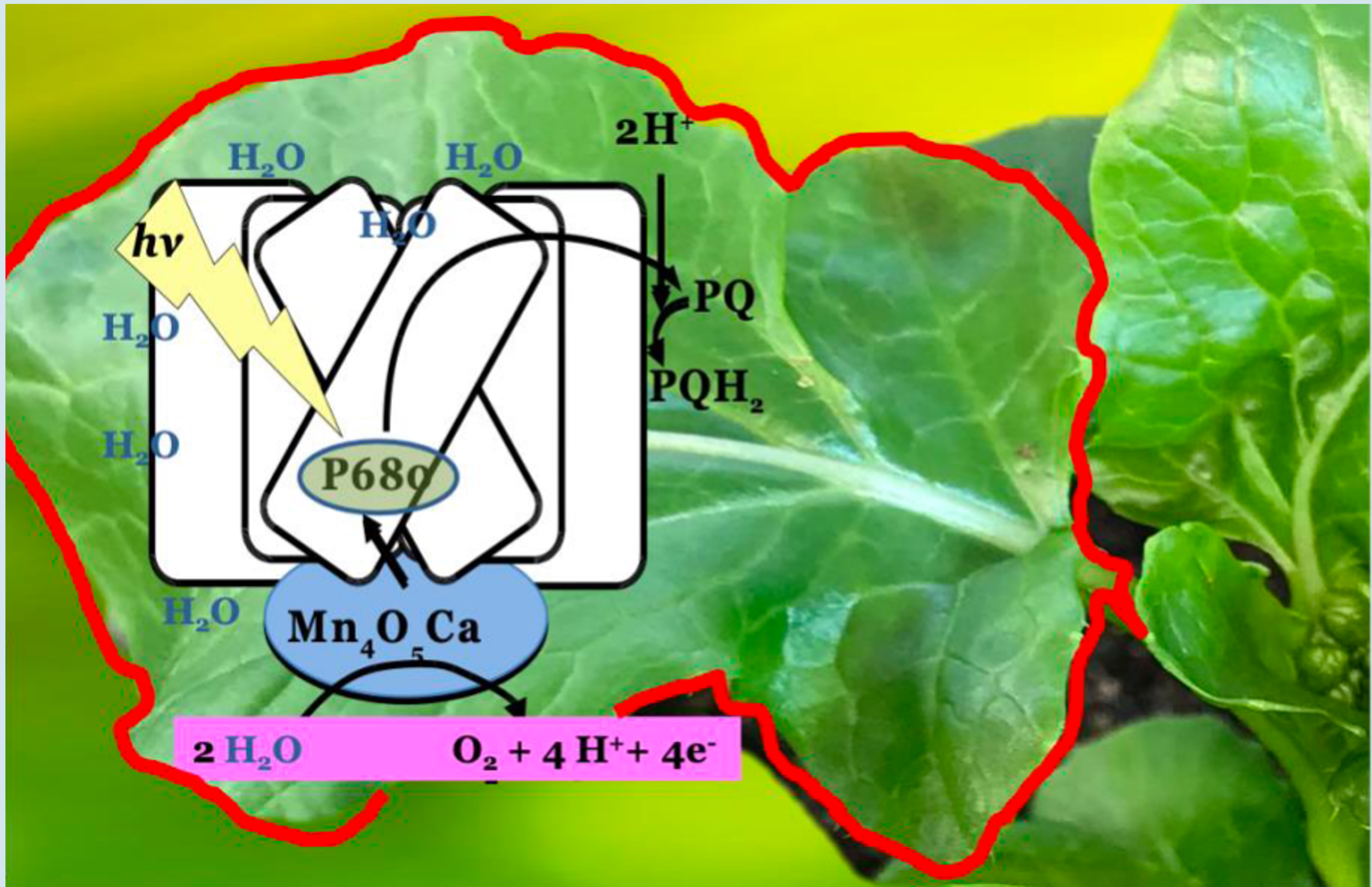
How are fluorescence and water mechanistically linked?

Water dynamics and the signal of fluorescence:

- The focus on water for photosynthesis is the photolytic process at the oxygen evolving complex

- Chl *a* Fluorescence as result of energy partitioning and light reactions is widely studied but information on the intrinsic relation of water and chlorophyll *a* is sparse

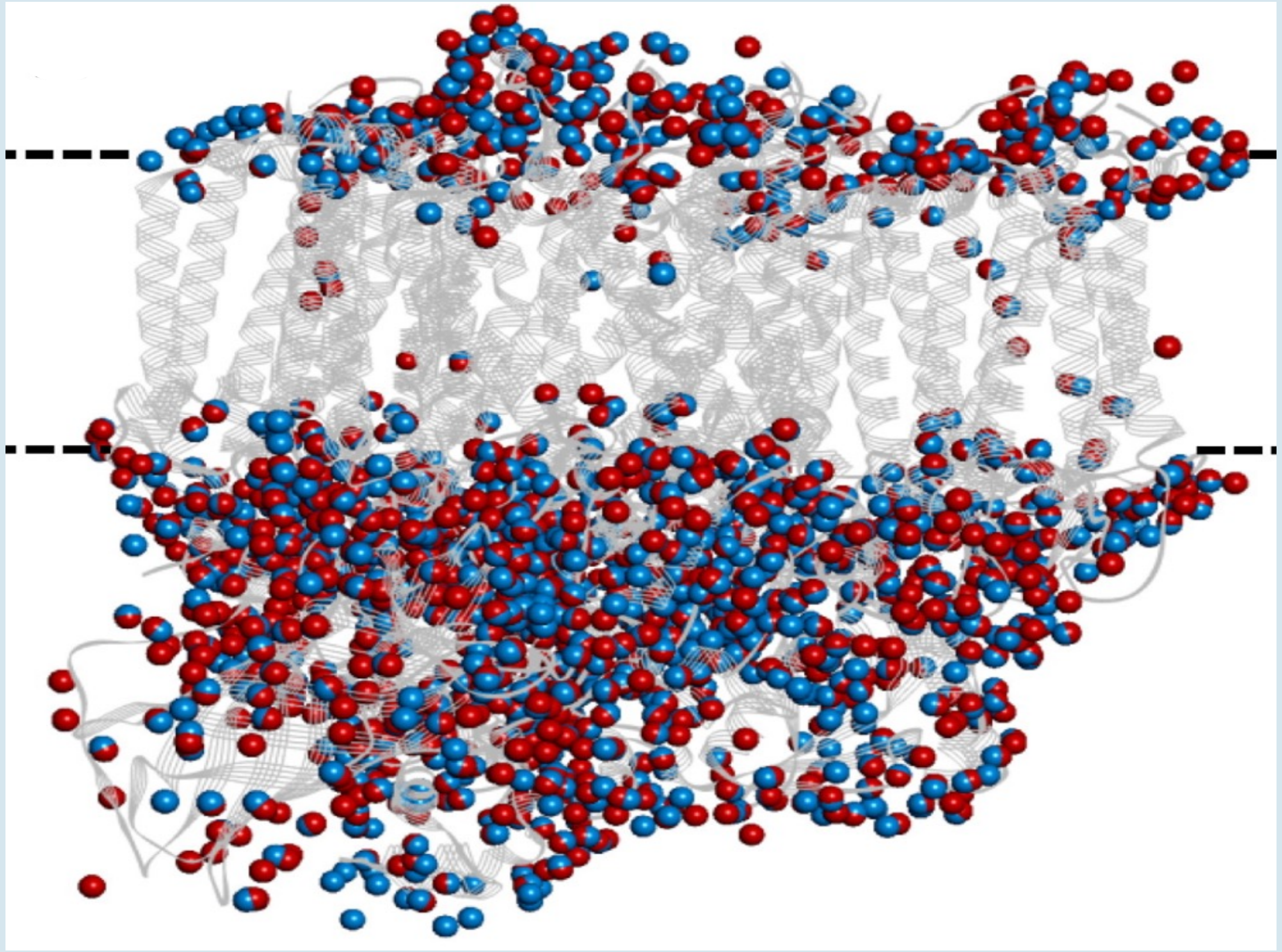
- Water is often considered a mere solvent or a disturbance for some techniques



Water dynamics at one single Photosystem II (PSII) level:

- The revolution in structural biology has allowed high resolution structures of the photosynthetic apparatus and just in and around one single PSII there are ~300K water molecules of unknown function

- Intriguingly, some of these waters are more bound (red dots) than others (blue dots)



Linke & Ho, 2013

PSII Crystal structure in cyanobacteria

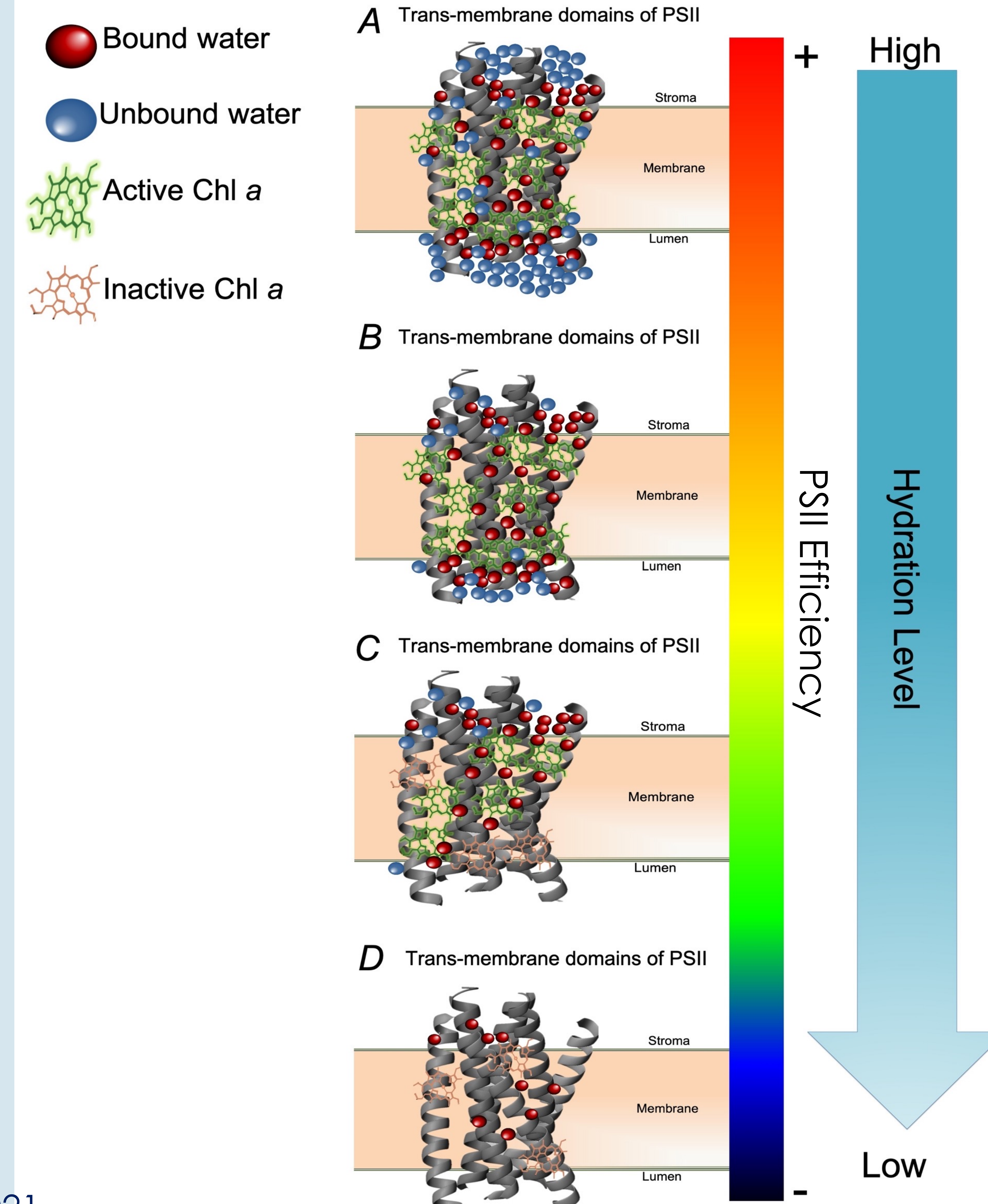
Hypothesis:

- *Water molecules have a mechanistic role in the complex's response to the environment*

➢ Are they cross-species aminoacidic differences that correlate to drought resistant phenotype?

➢ Do these differences affect fluorescence dynamics?

Guadagno *et al.* – Photosynthetica, 2021

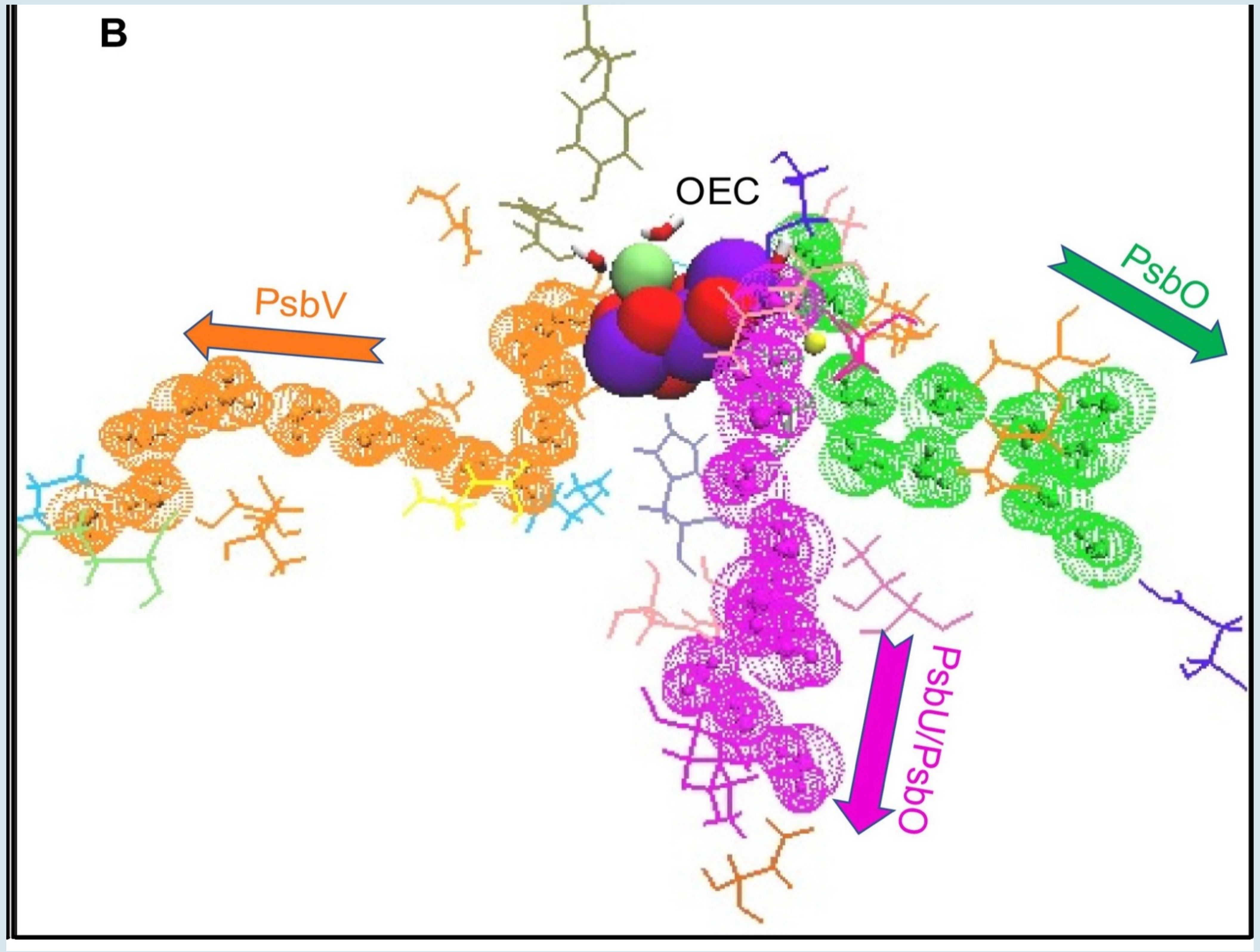


Water Channels Analysis:

- Characterize electrostatic interactions *via* MCCE across species
- Studying water channels/angles under different pressure and temperature to simulate different hydration levels of PSII (plants)
- Transcriptomic-informed "mutated" crystal structures in the aminoacidic chains for PSII and beyond - downstream

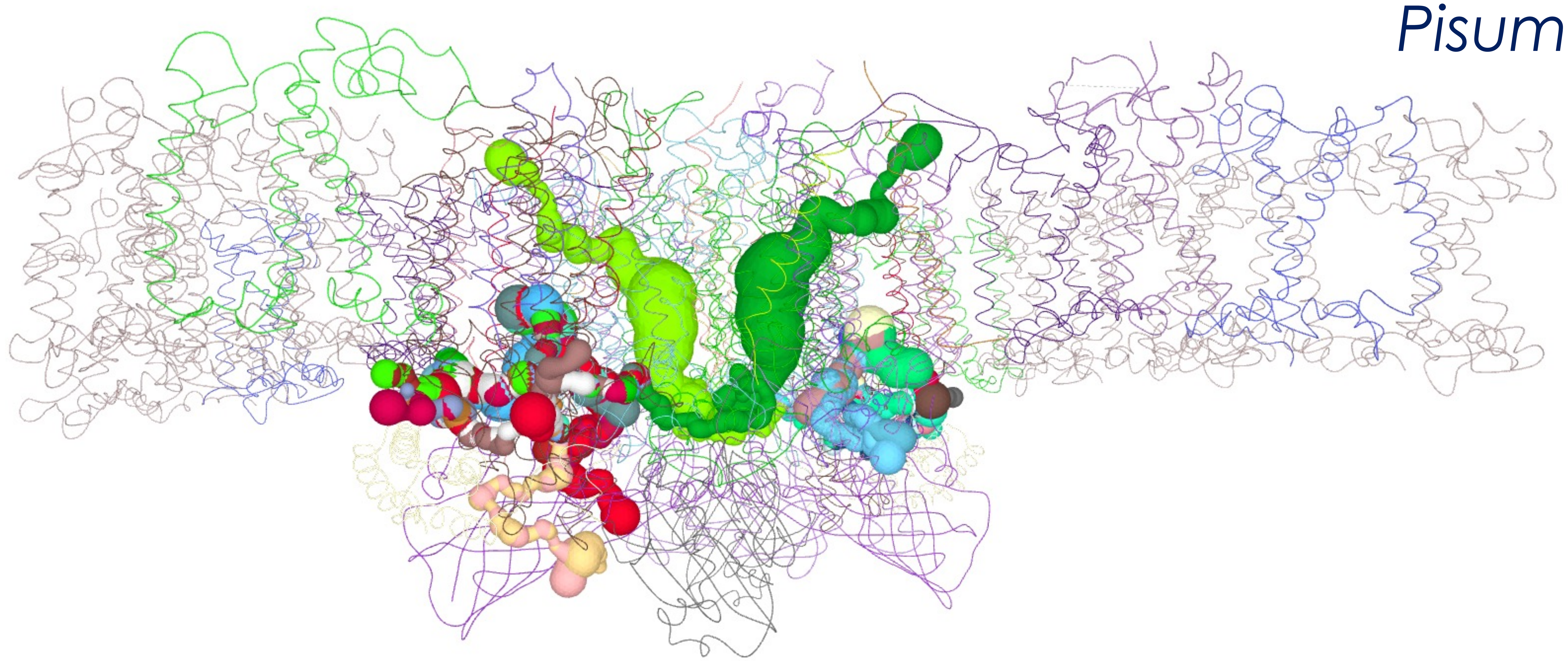
Ben Romanjenko (UW)

Marilyn Gunner Lab (CCNY)

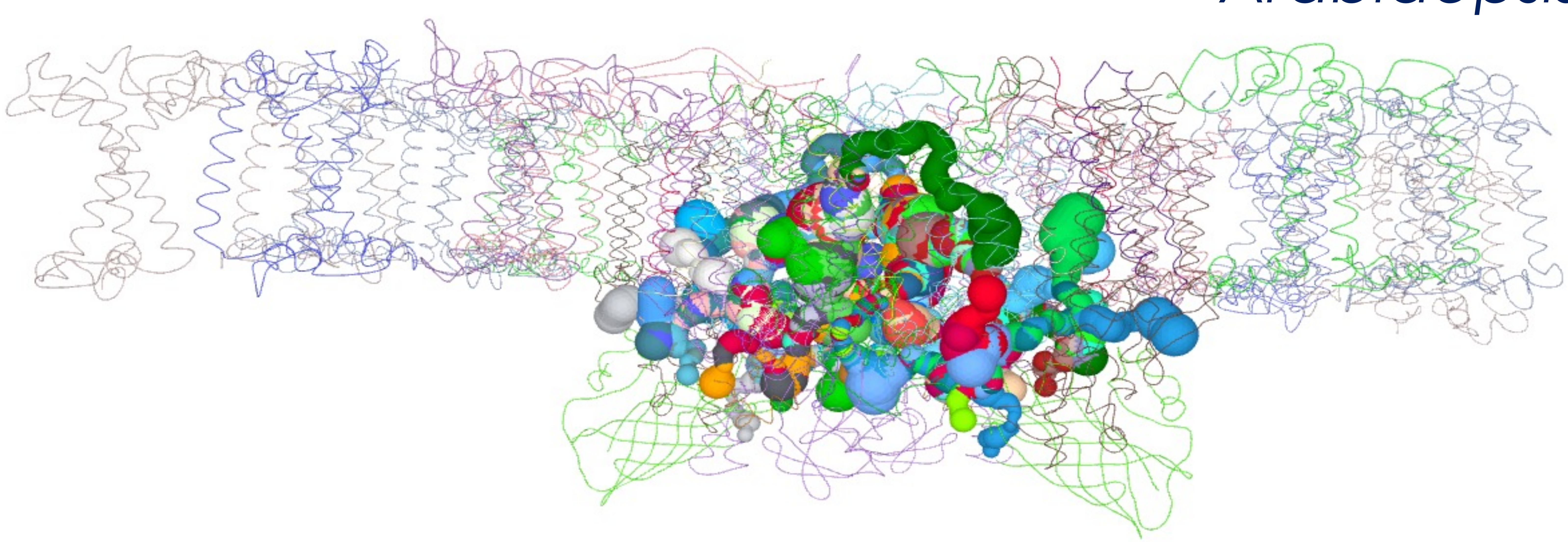


Cross-species water channel characterization:

Lateral profile
Pisum sativum



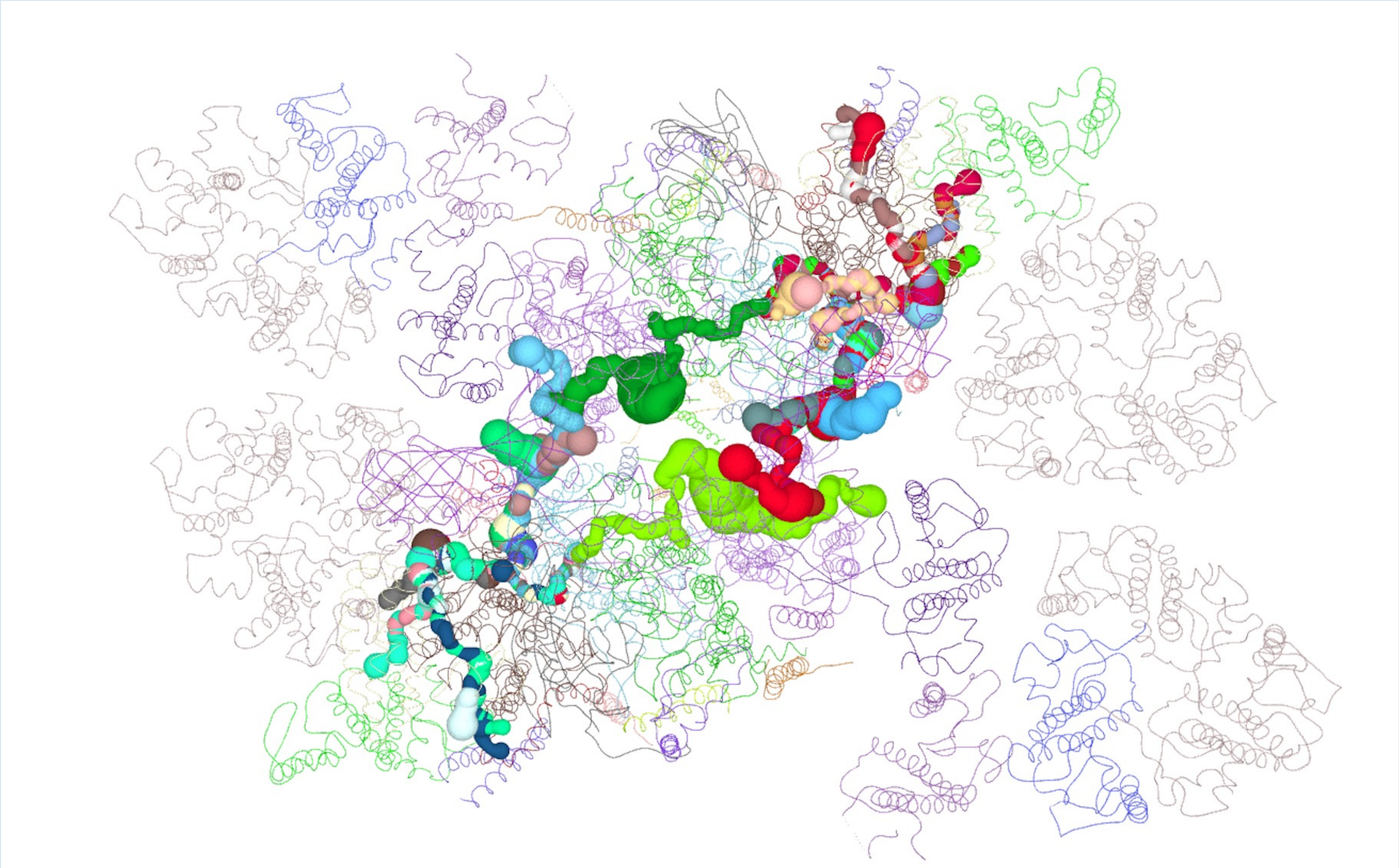
Lateral profile
Arabidopsis thaliana



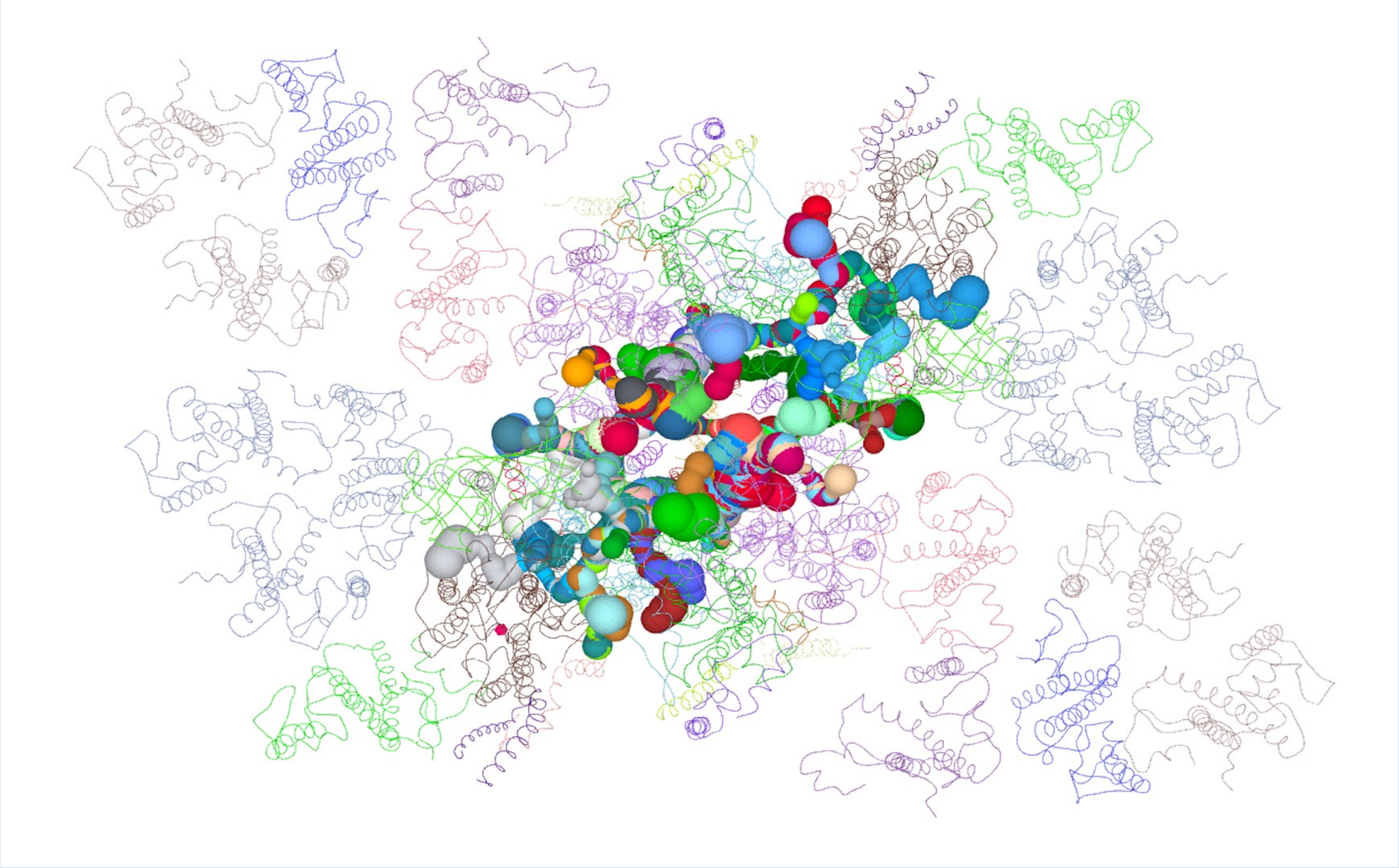
Structure resolutions are 2.79 A and 2.7 A. The closest resolutions available

AG2PI
Agricultural Genome to Phenome Initiative

Cross-species water channel characterization:



Luminal profile
Pisum sativum



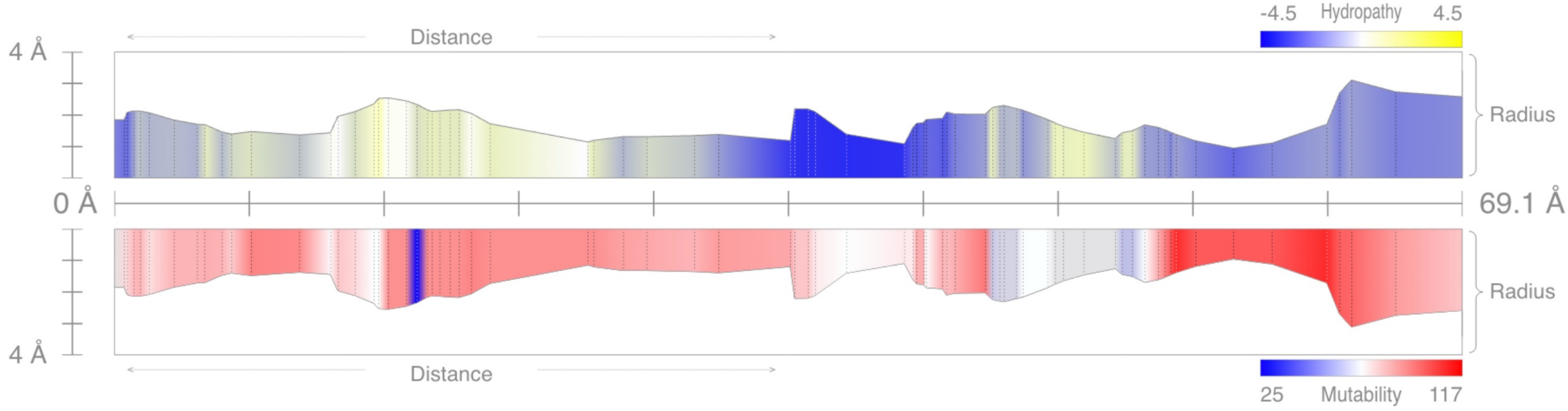
Luminal profile
Arabidopsis thaliana

Not many available
High-res structures

Agricultural Genome to Phenome Initiative

Cross-species water channel characterization:

Pisum sativum



Arabidopsis thaliana

AG2PI Agricultural Genome to Phenome Initiative

Can we correlate up with the phenotype and down to sequence?

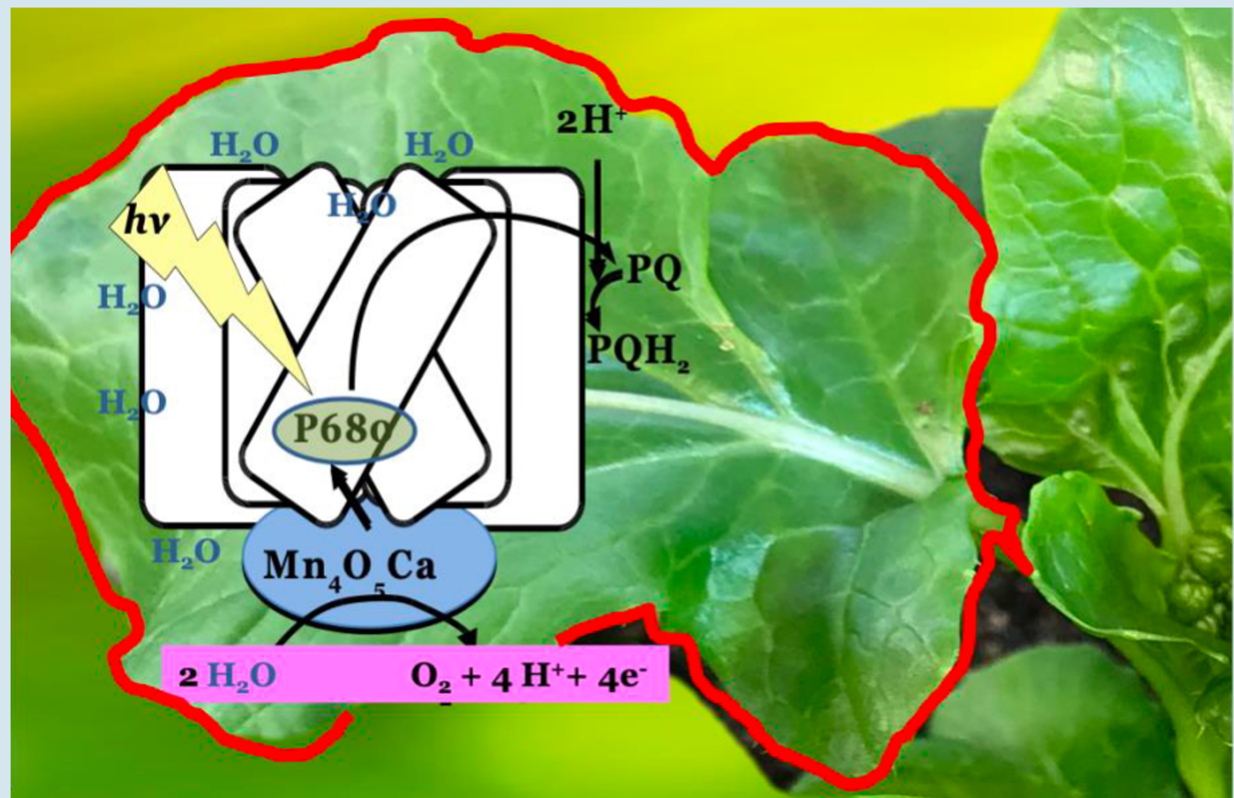
How to test our hypothesis:

Dave Hanson (UNM)

- **Molecular Biophysical Simulations – Molecular Dynamics**
- Use of Mutants
- **Spectroscopic investigations**
- **MicroNeedle-type *in situ* plant water content sensors**
- 3D - microCT scans of plant tissue

Tania Tibiletti
CEA - Saclay (France)

FA FOUNDATION



Expected Research Impacts of PSII water dynamics:

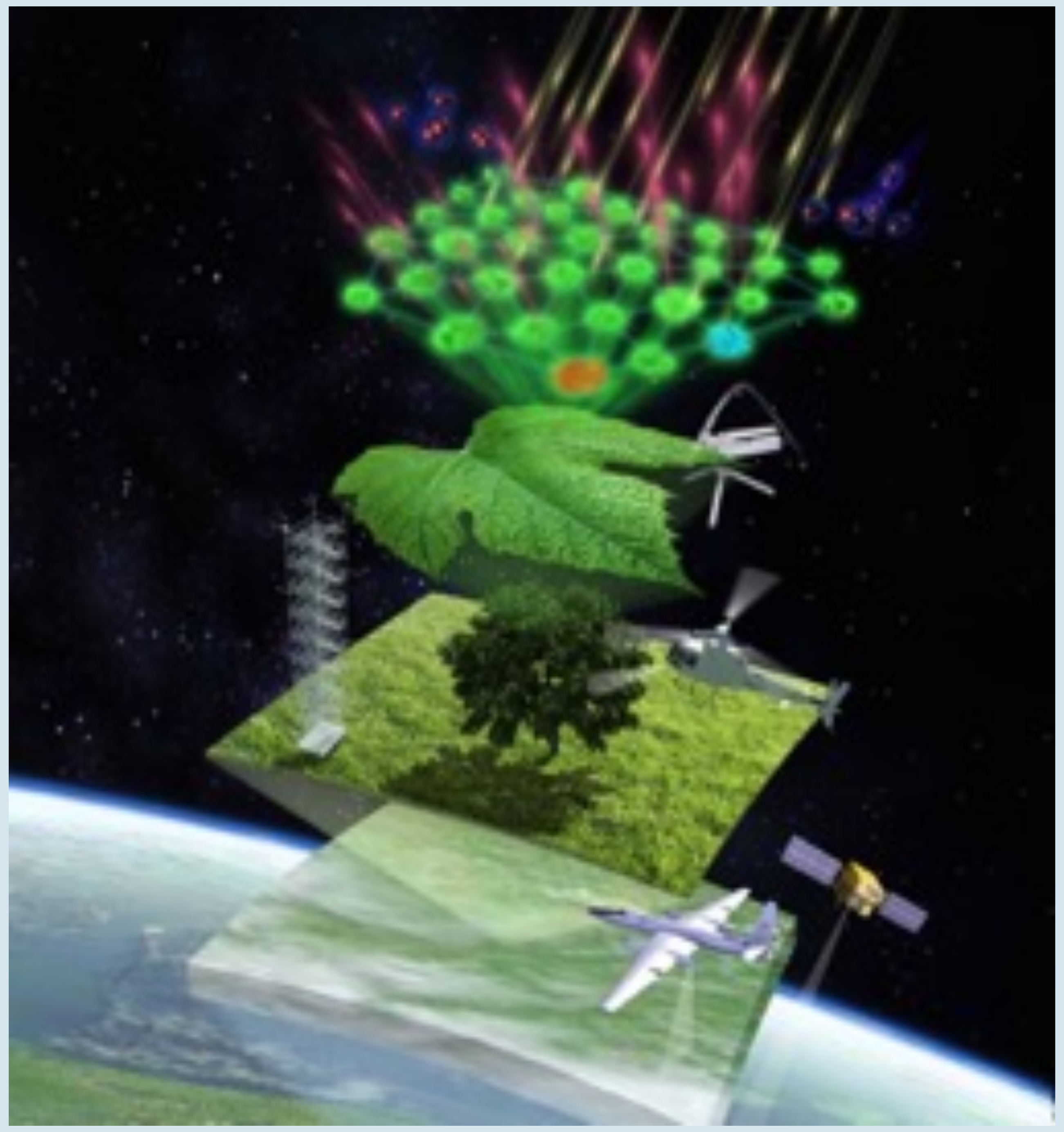
- Improved mechanistic understanding of chlorophyll *a* fluorescence, a current widely used proxy of plant vigor

- Insights on "easily" scalable chemical potentials at the base of several leaf-level eco-physiological measurements (e.g., leaf water potential, impedance)

- Relevant to genotypic and species variation and applicable to any type of stress response (e.g., temperature changes, pH)

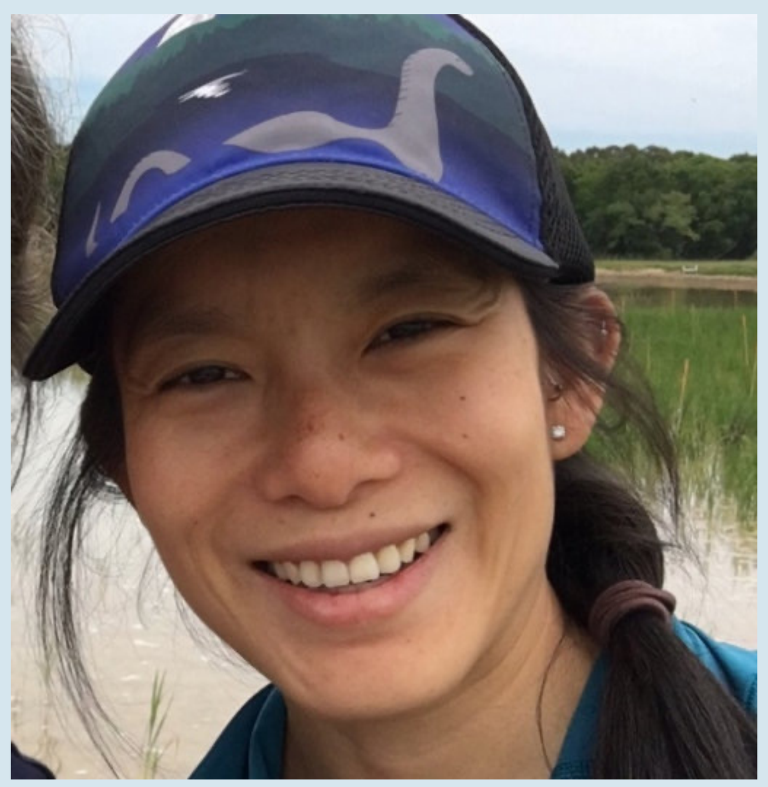
Informed Phenotyping – based on cross-scale mechanistic relations

http://web.gps.caltech.edu/~cfranken/research.html



Plant Genome Research Program (PGRP)#2102120

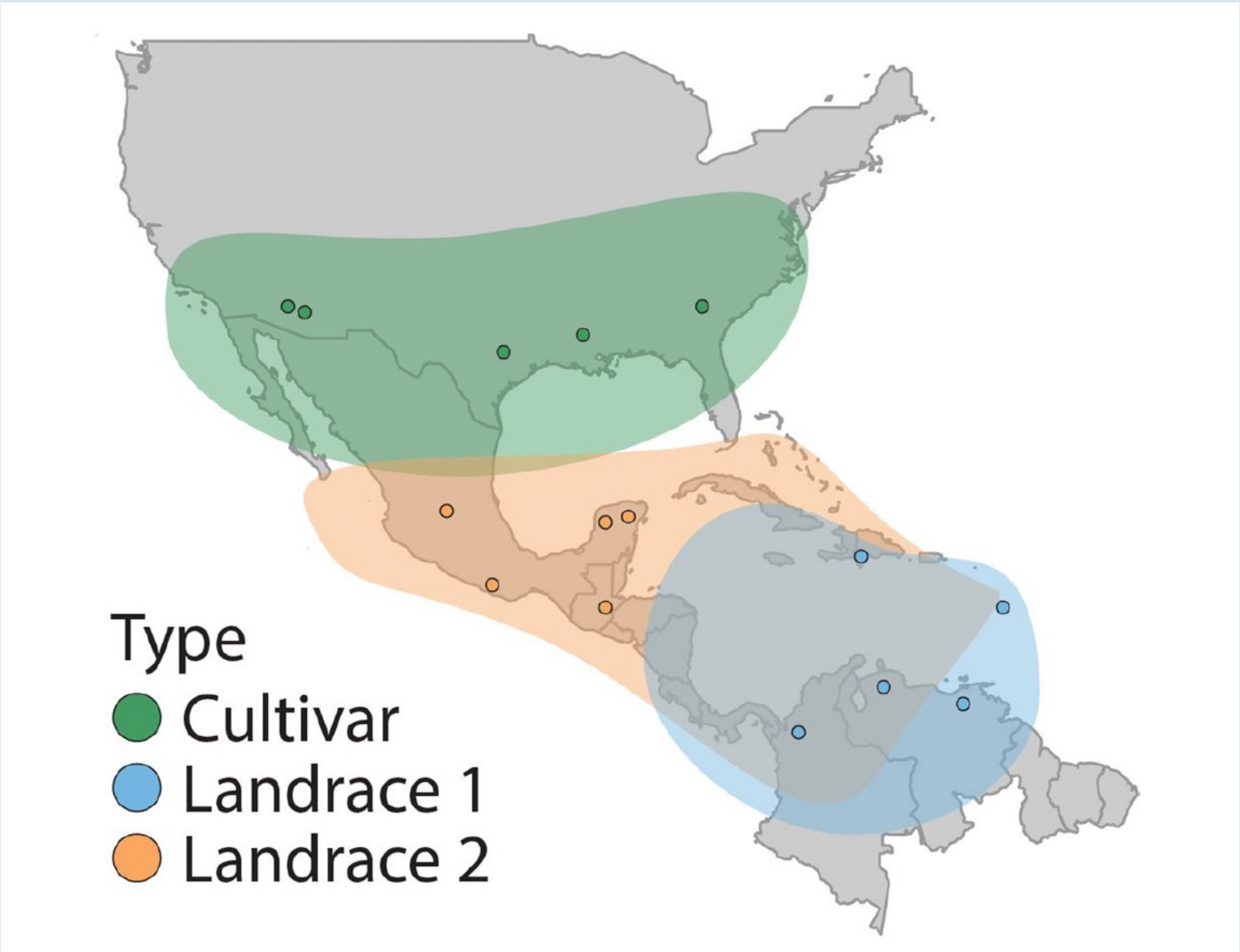
Duke Pauli (University of Arizona)

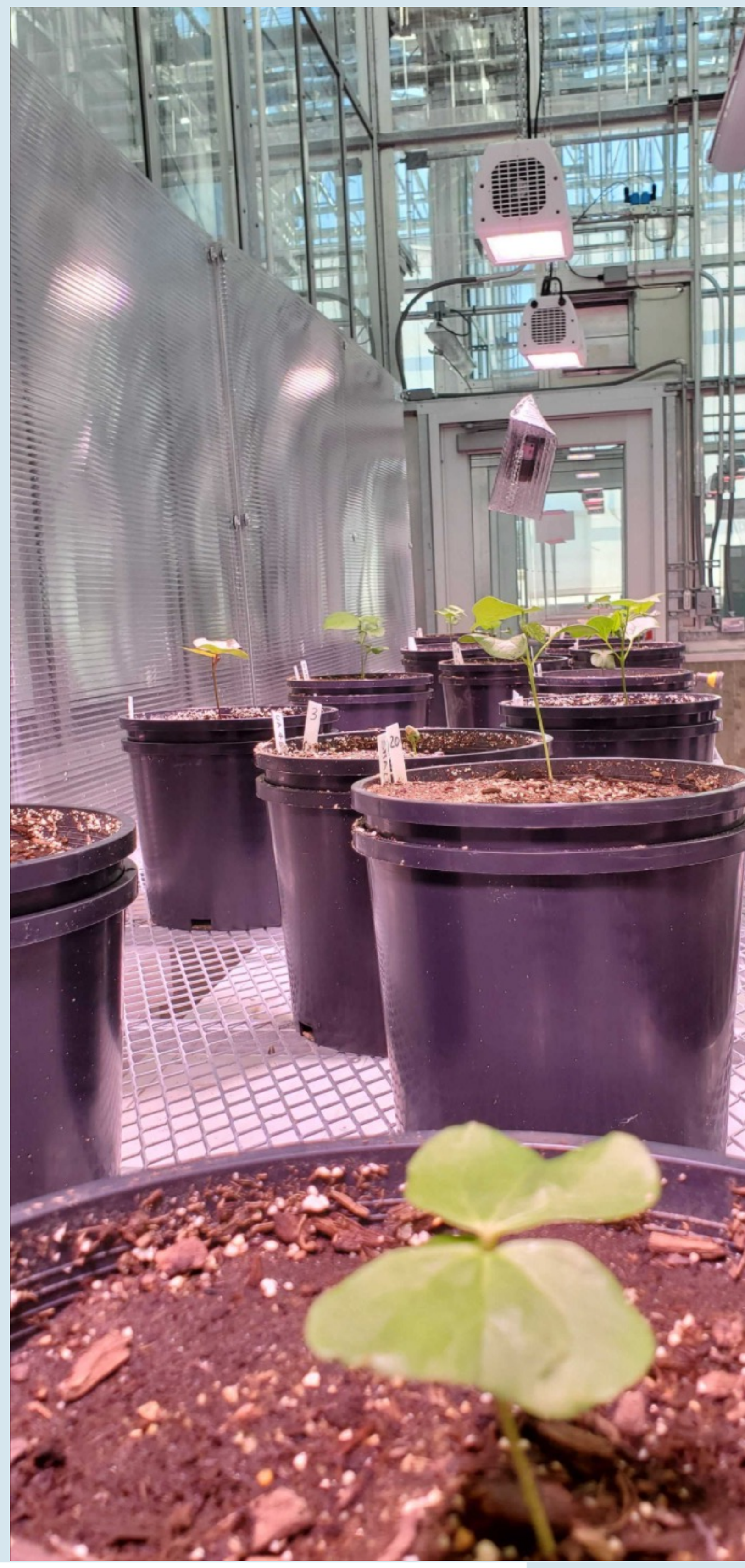


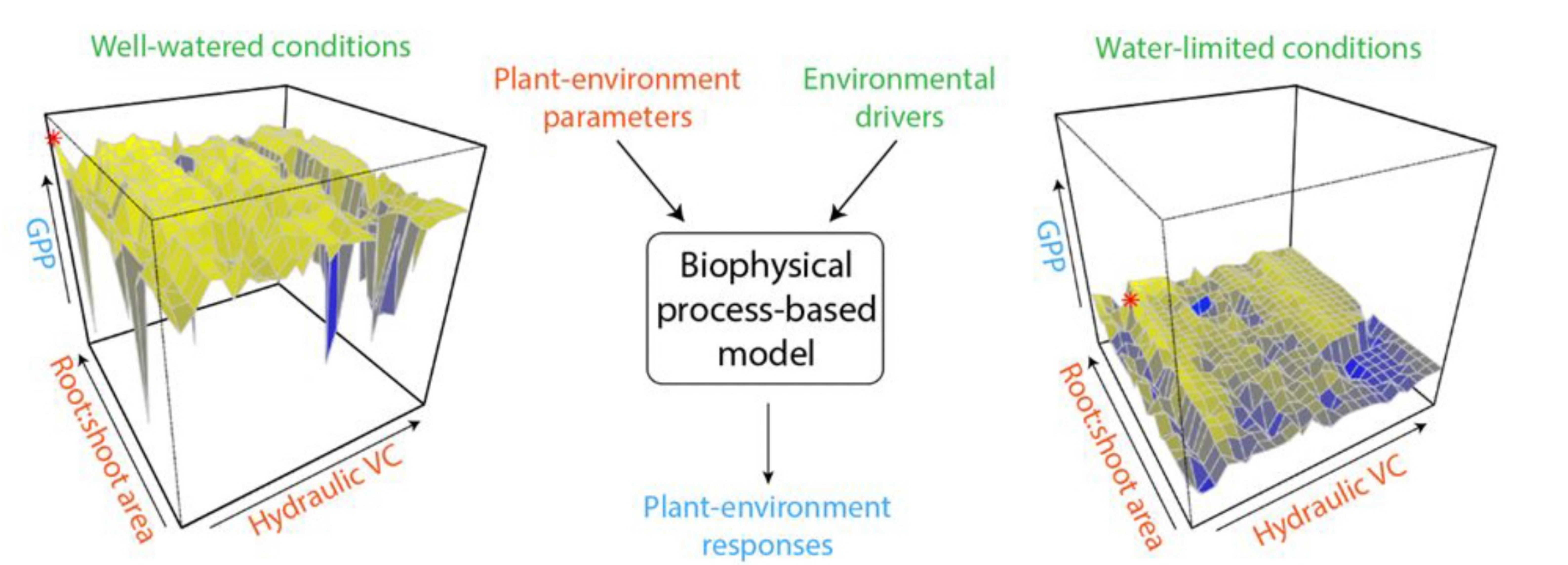
Diane Wang (Purdue University)

Andrew Nelson (BTI)

Joshua Udall (USDA)







Utilizing biophysical models (BPMs) to explore genetic fitness landscapes. Simulation results of gross primary productivity (GPP) across a grid of parameter combinations using TREES in two environmental scenarios (left: well-watered, right: water-limited). Parameters representing 25 different hydraulic vulnerability curves (VCs; represented here in units of -MPa by the xylem potential at 50% conductivity loss) and 25 values of root to shoot area ratios were explored, totaling 625 parameter combinations. VC values were selected based on a range determined empirically [52] while root to shoot ratios were varied +/-10% from previous simulations on cotton. Red star in each plot indicates the global maximum.

In the future:

- **Possible implementation of ecosystem models using biophysical first principles of energy partitioning at PSII level – less empiricism**

- **Improved predictions of changes in energy balance for productivity, stress response, recovery and mortality under unknown future environmental conditions**

More inter-disciplinary work is needed to study cross-scale phenomena