AEROGELS AND HOW TO TAILOR THEM FOR PHOTOCATALYSIS

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INTRODUCTION

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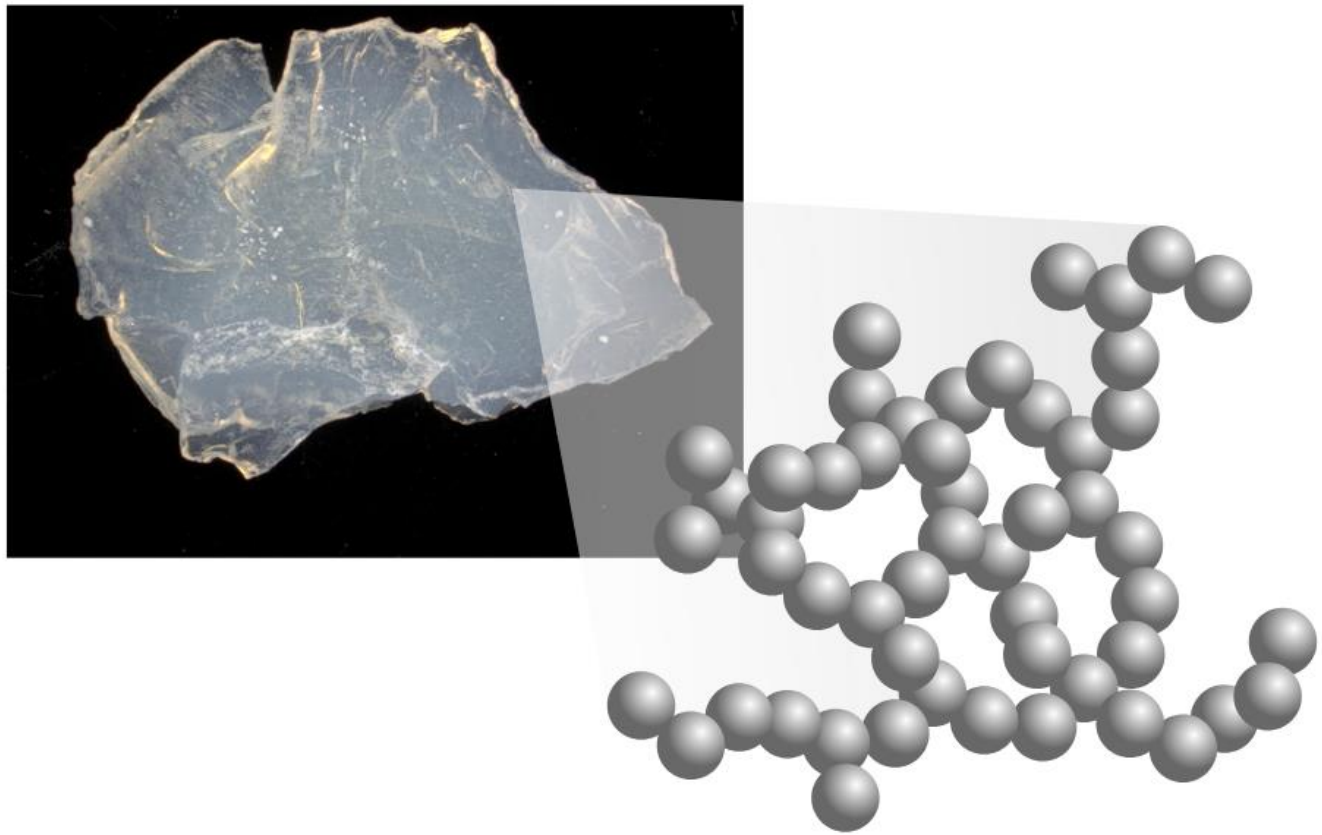
Aerogels?

- Highly porous matter
  - Oxides
  - Polymers
  - Carbon
- Large inner surface
- Controlable pore sizes
- Ultra low thermal conductivity



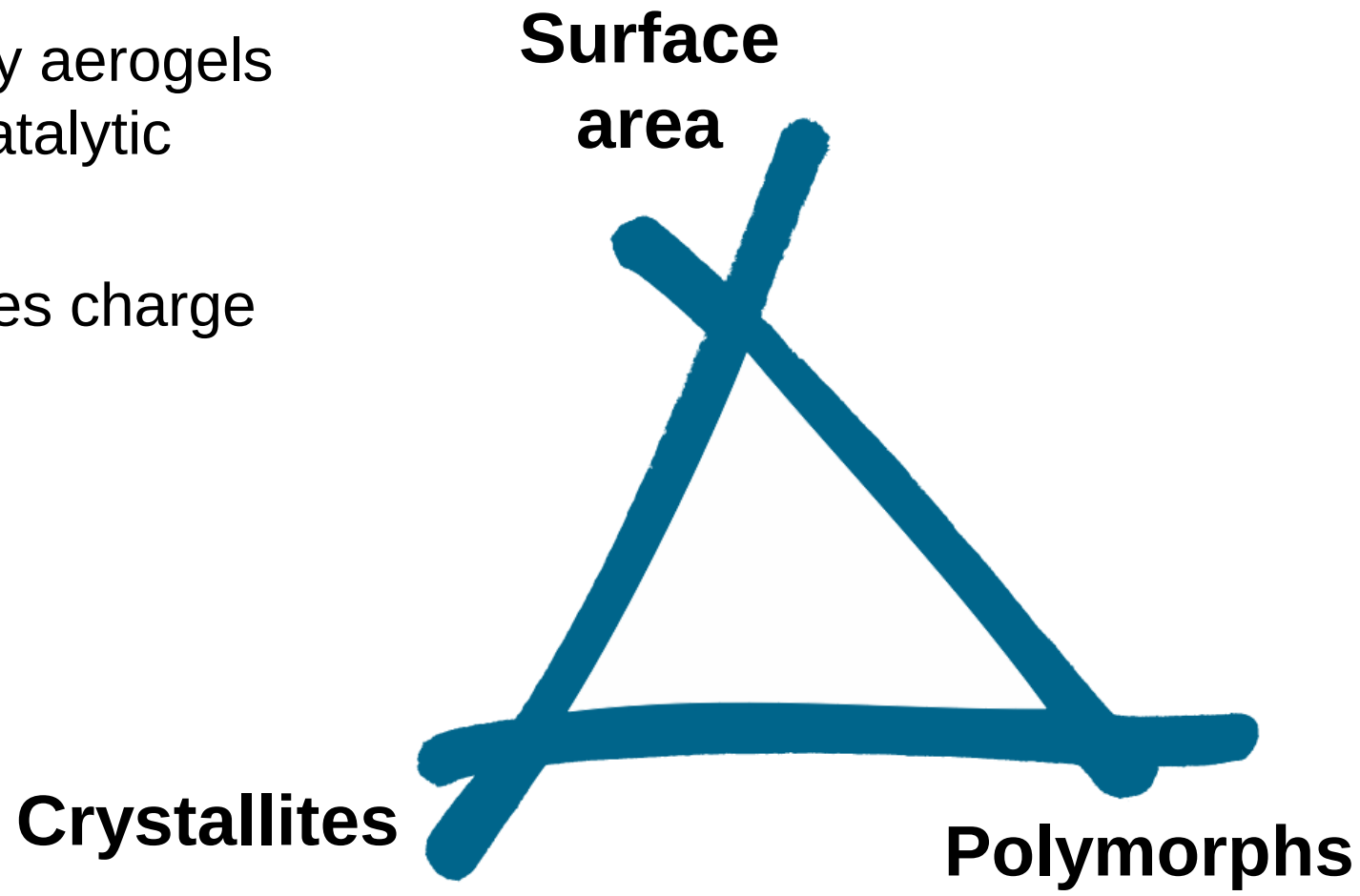
Photography: A. Rose

Introduction and Motivation
Aerogels and Aerogel Composites

- Aerogel related research in the fields of
  - Transport
  - Energy
  - Aviation
  - Space
  - Sustainability

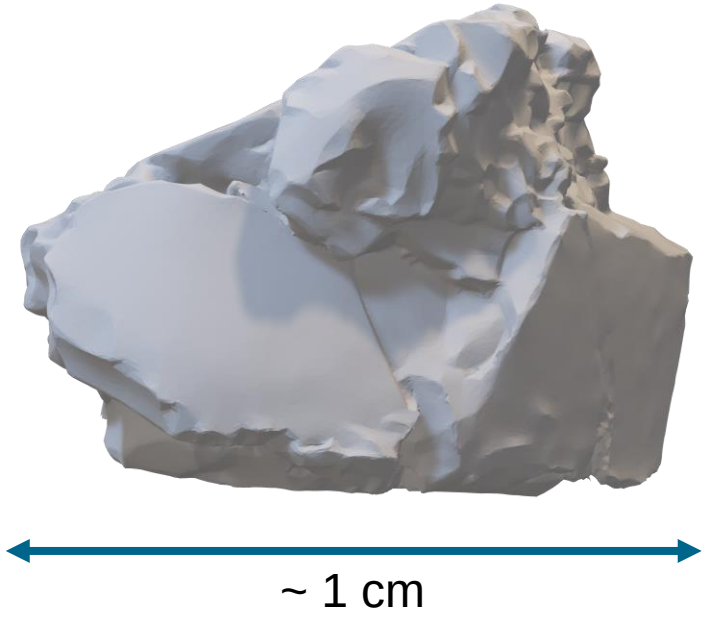
Introduction and Motivation
Potentials of Semiconducting Aerogels

- Large surface areas provided by aerogels could be beneficial for (photo)catalytic activities
- Interconnected network promotes charge carrier transport
- Potential applications:
  - Green hydrogen production
  - VOC degradation
  - Nitrogen reduction reaction



Goal

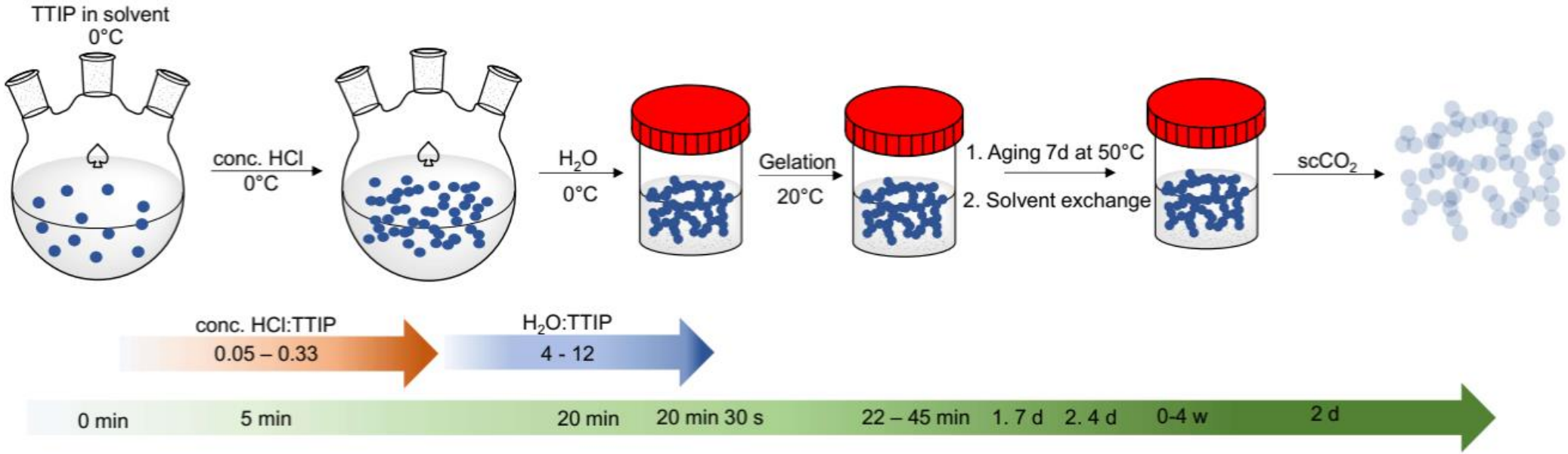
- What are the suspected optimal properties?
  - High degree of crystallinity
  - Large specific surface area
  - Transparency
  - Recyclability
  - (Low process costs)



RESEARCH RESULTS

Synthetic Protocol

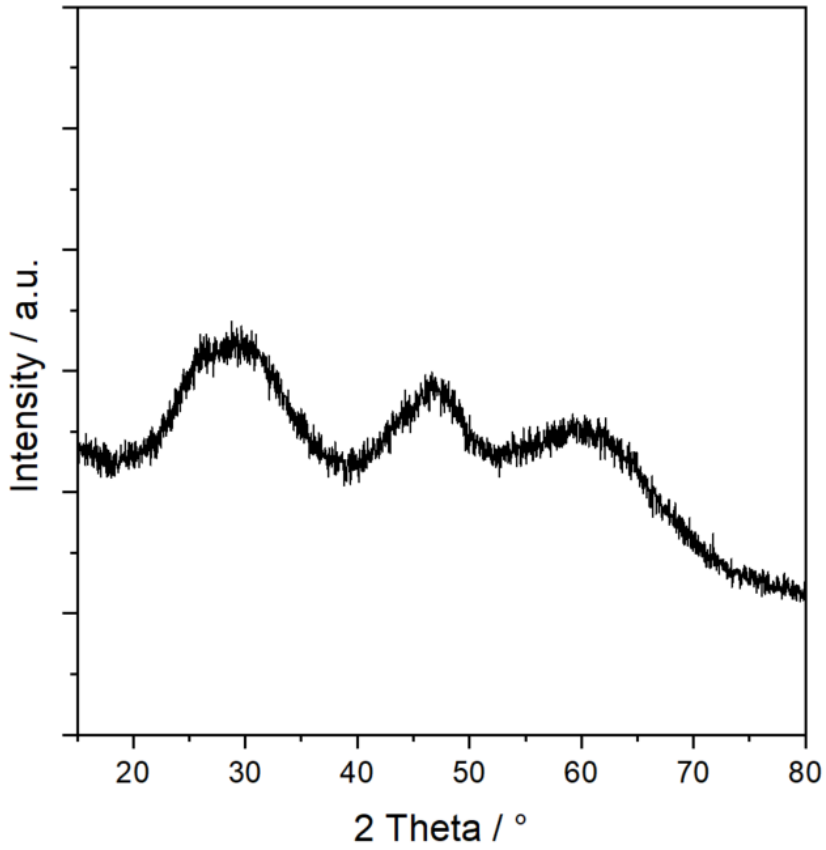
- How to make highly porous titania:



TTIP: Titanium tetraisopropoxide

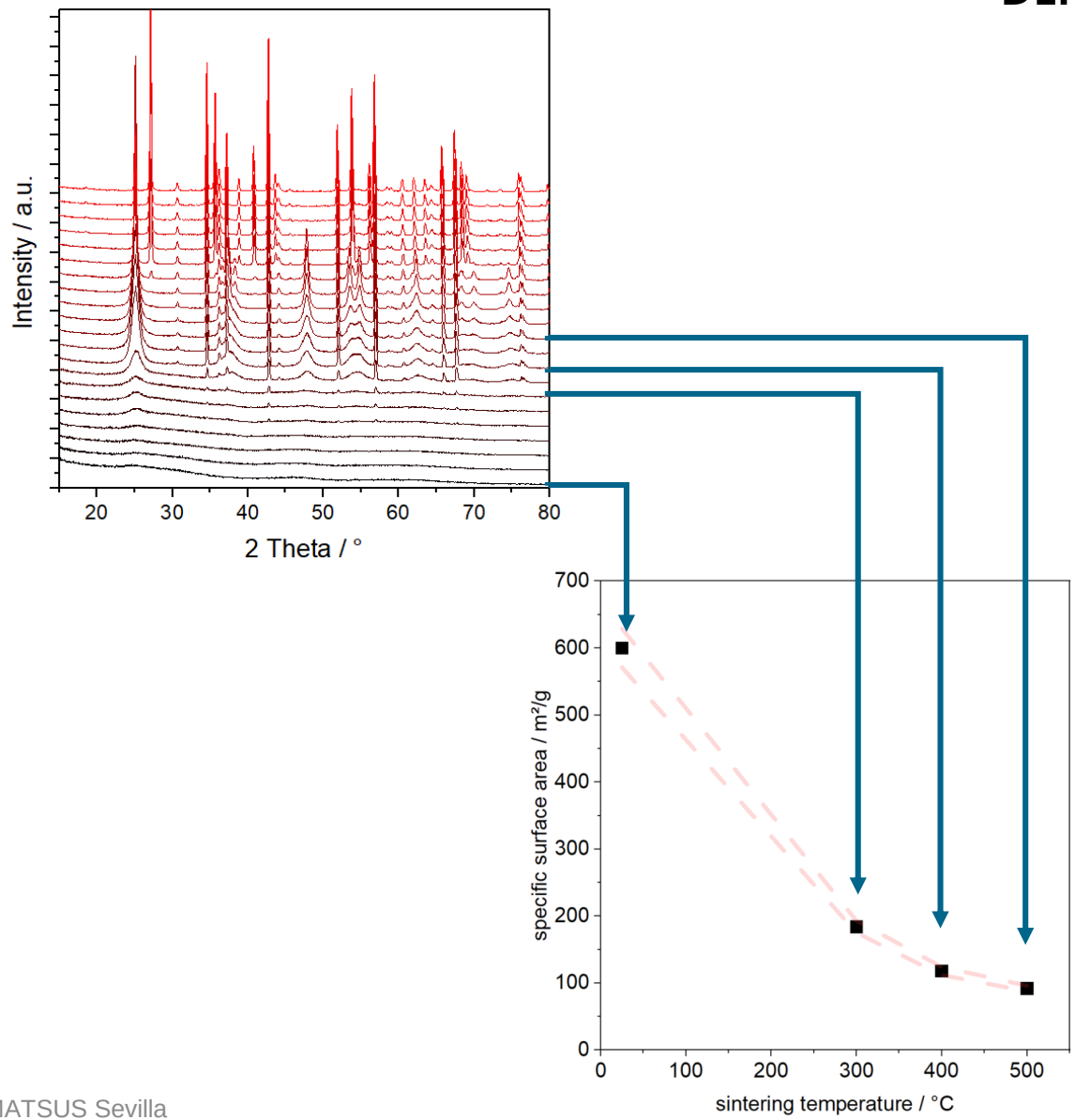
Thermal Conversion of Polymorphs and Surface Area

- Developed standard protocol leads to amorphous titania
- No specific reflexions visible
- Halo of amorphous matter



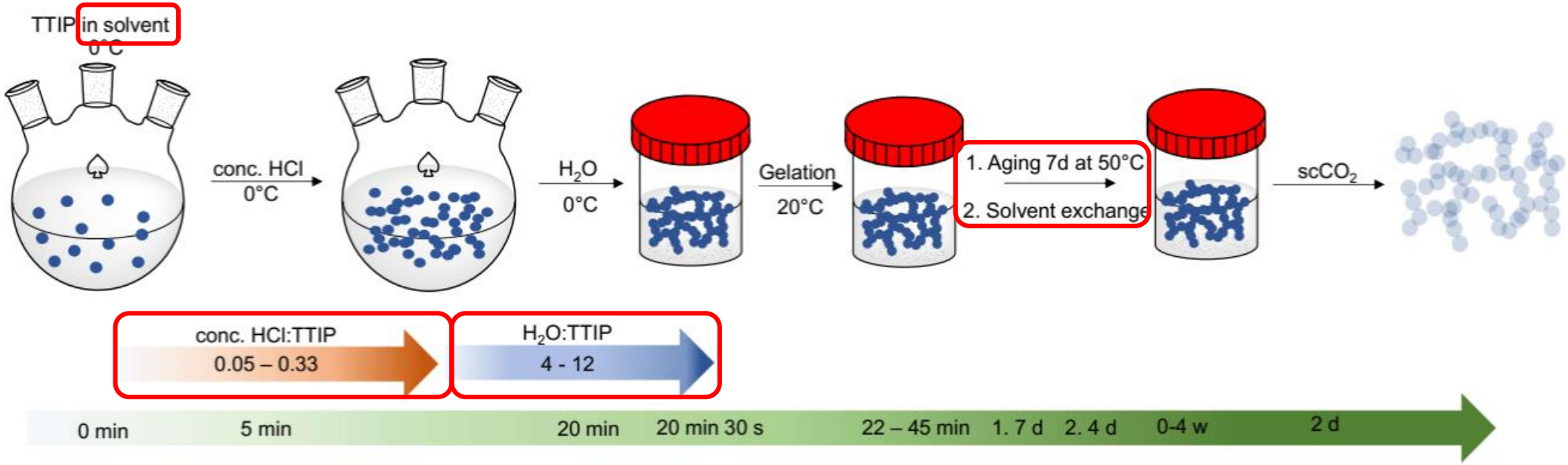
Thermal Conversion of Polymorphs and Surface Area

- Pristine aerogels can be transformed into anatase and rutile
- Surface area is drastically decreased due to sintering
- **Direct induction of polymorphs possible?**

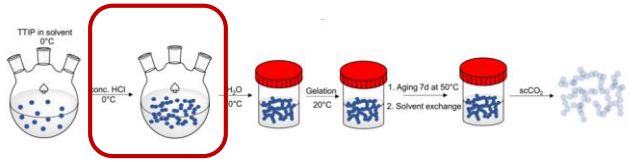


Synthetic Strategy – Tuning Parameters

- Parameter variation and process window optimization



Optimize Crystallinity



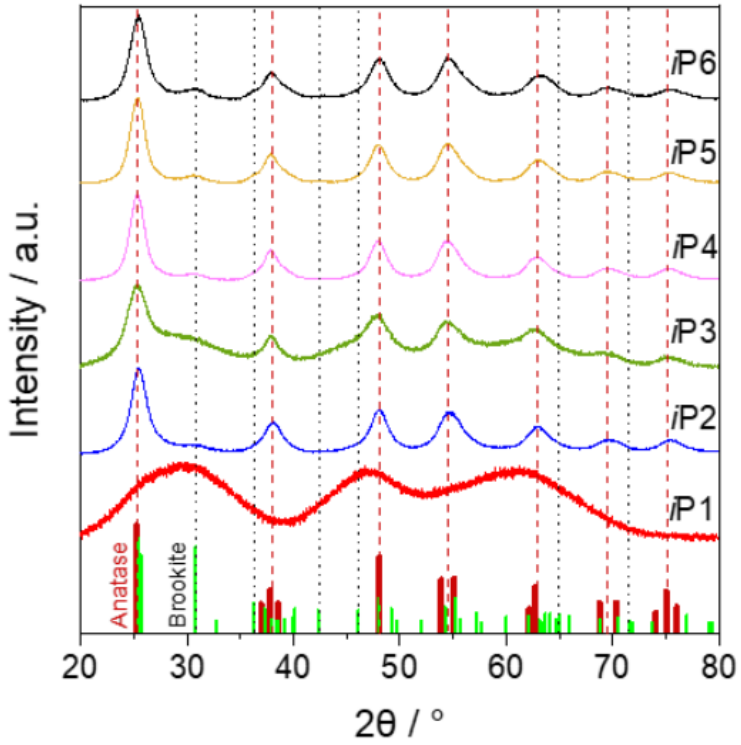
Increase HCl concentration

Increase H_2O concentration

Increase aging time

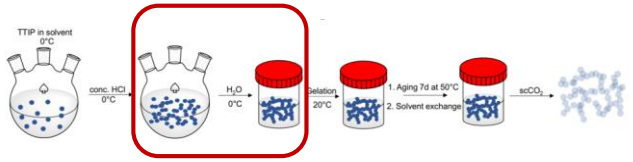
Side effects:

- Formation of secondary phase
- Lower surface area, larger pores, broader pore size distribution, lower pore volume



Sample	Crystallinity / wt.%	Phase content / wt.%	Crystallite size / nm	S_{BET} / $m^2 \cdot g^{-1}$
*i*P1	amorphous	-	-	554 ± 26
*i*P2	44 ± 0.4	A	4.3 ± 0.05 (A)	536 ± 26
*i*P3	54 ± 1	A	5.4 ± 0.09 (A)	586 ± 28
*i*P4	94 ± 5	64 ± 0.6 (A)+36 ± 4.6 (B)	5.4 ± 0.07 (A),2.2 ± 0.13 (B)	266 ± 13
iP4.1	100 ± 3	58 ± 0.6 (A)+42 ± 3.4(B)	5.0 ± 0.07 (A),2.8 ± 0.14(B)	280 ± 13
*i*P5	94 ± 3	61 ± 0.4 (A)+39 ± 2.8 (B)	5.3 ± 0.05 (A),2.4 ± 0.13(B)	211 ± 10
*i*P5.1	100 ± 2	58 ± 0.7(A)+42 ± 2.3(B)	4.7 ± 0.07(A),3.1 ± 0.13(B)	271 ± 13
*i*P6	100 ± 4	58 ± 1.7 (A)+42 ± 2 (B)	4.2 ± 0.06 (A),2.5 ± 0.08 (B)	307 ± 15

Optimize Crystallinity



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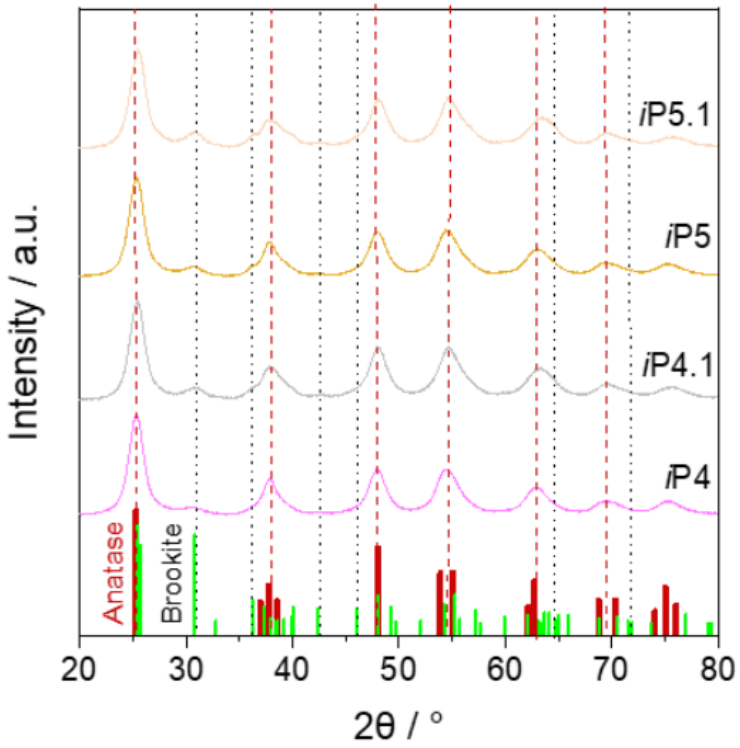

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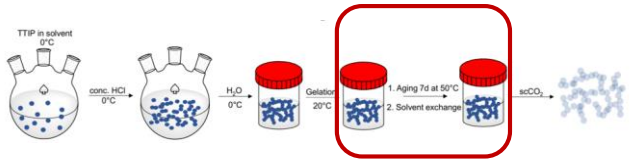

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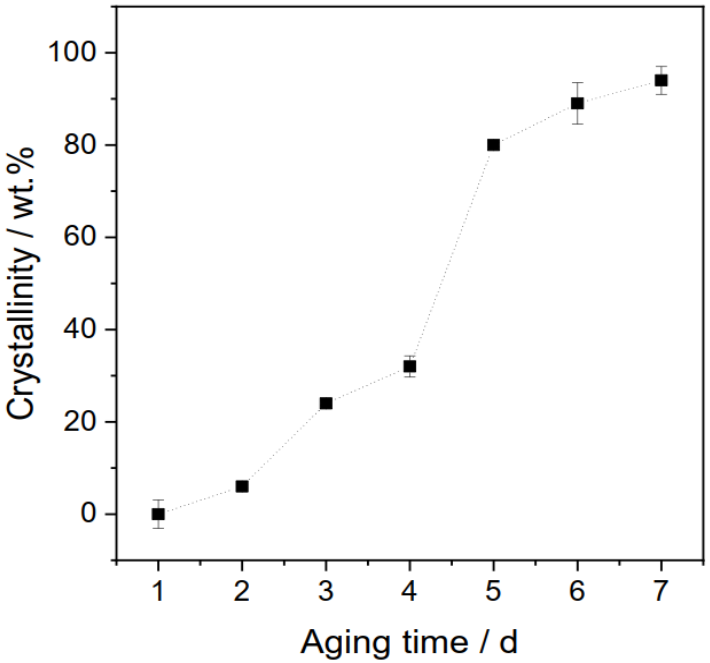

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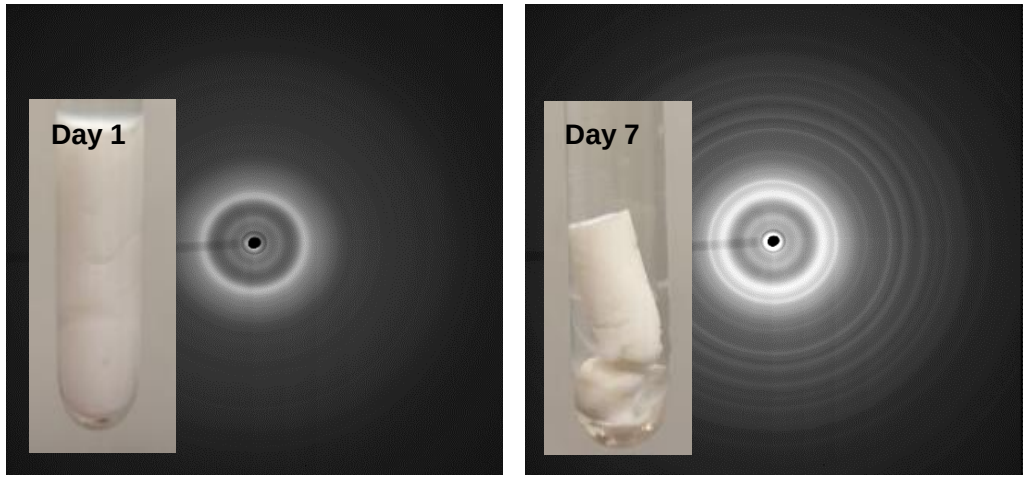

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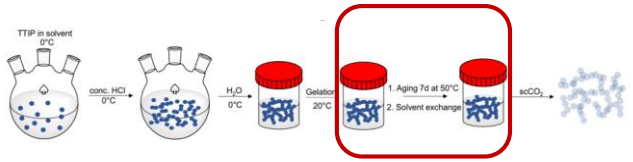

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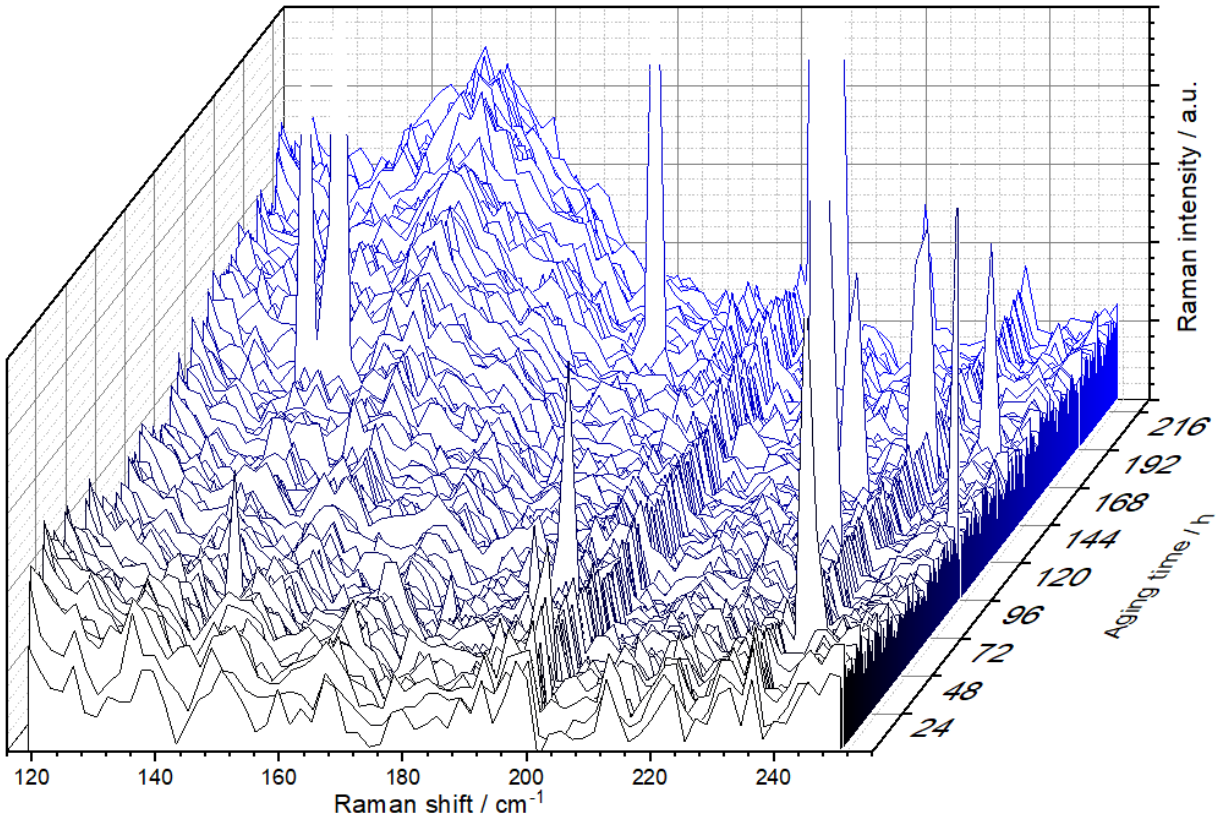

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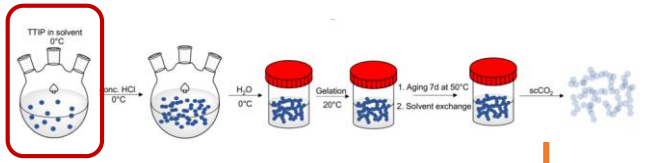
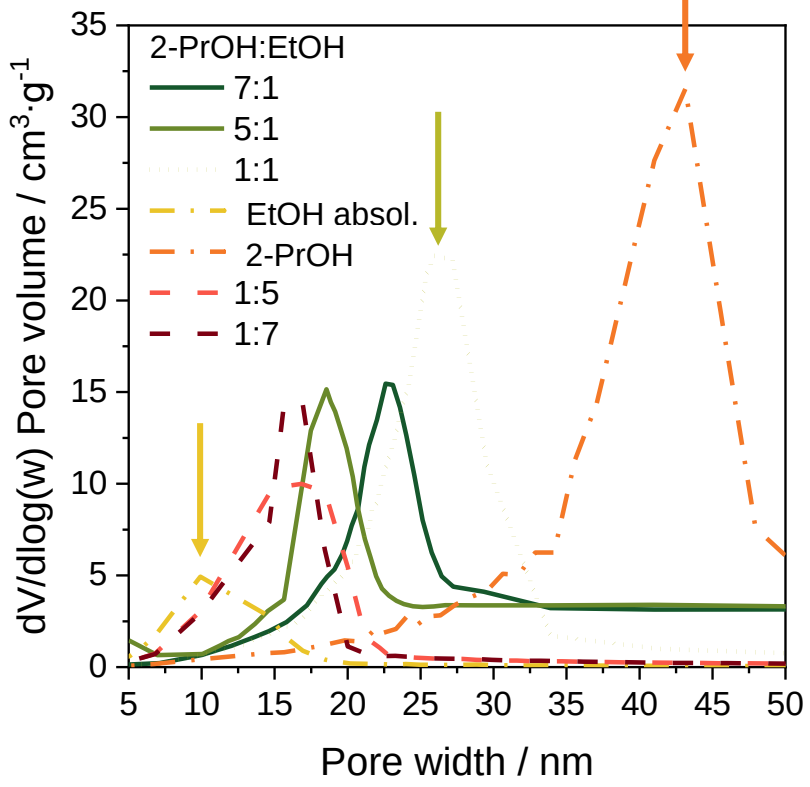
Tuning Pore Structure



Change solvent (mixture):

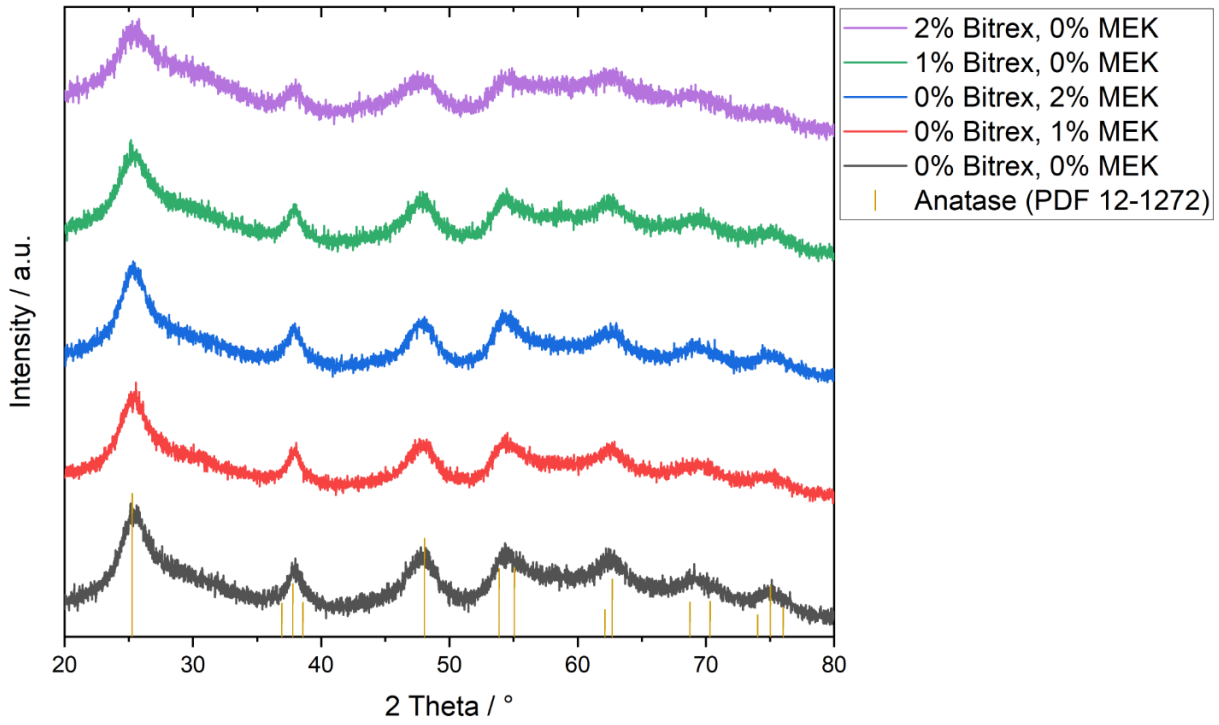
Increase 2-PrOH fraction ⬆

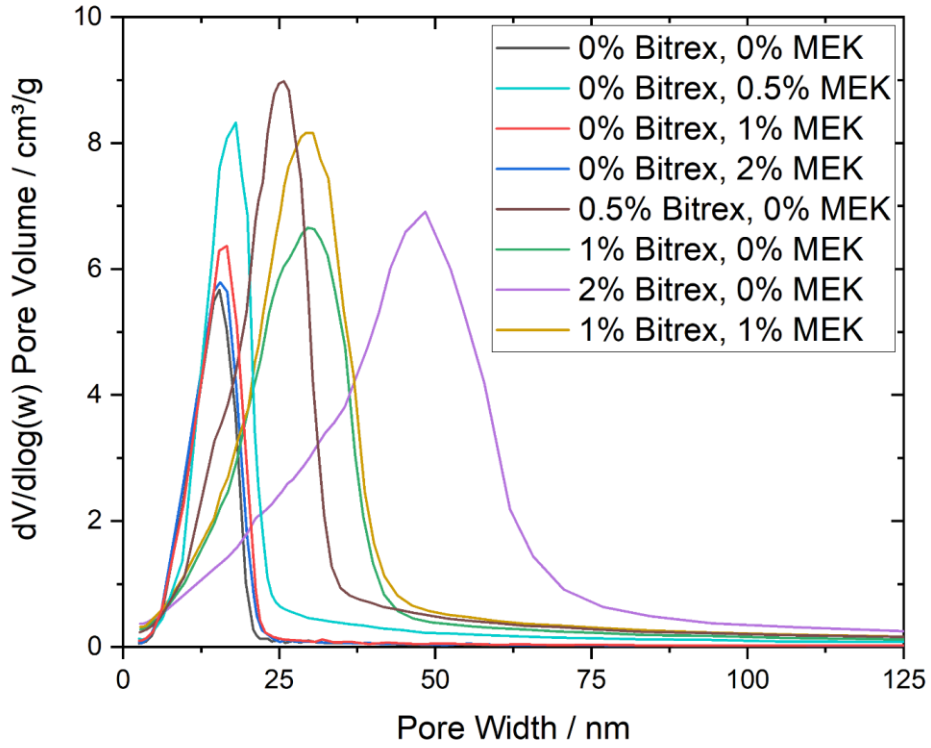
- Shrinkage increases
- Specific surface area increases (up to a ratio of 1:1)
- Pore sizes increase (except 2-PrOH:EtOH ratio of 1:1)
- Opacity increases, larger monoliths (except 2-PrOH:EtOH ratio of 1:1)
- Gelation time decreases (up to a ratio of 1:1)



Further Impact Factors

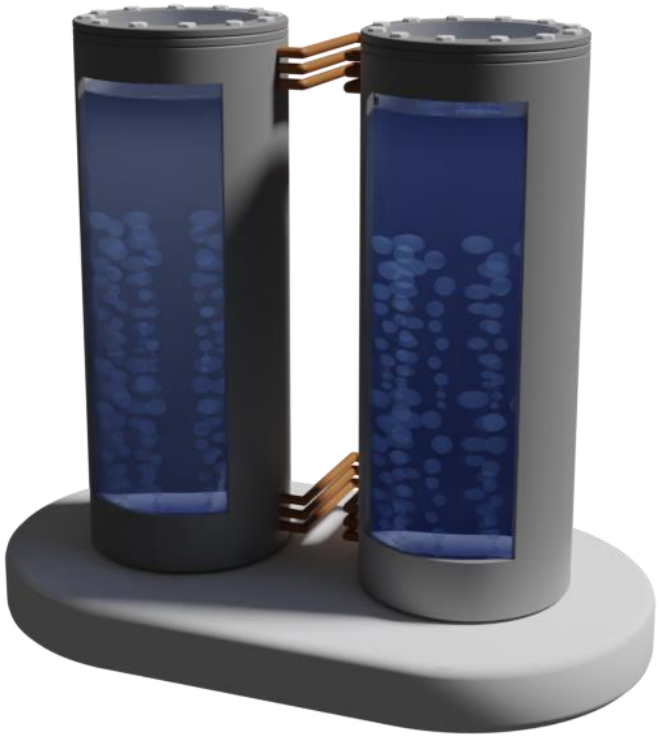
- Solvent exchange? → no influence found
- Denaturing agents in ethanol → Bitrex® causes alternating properties



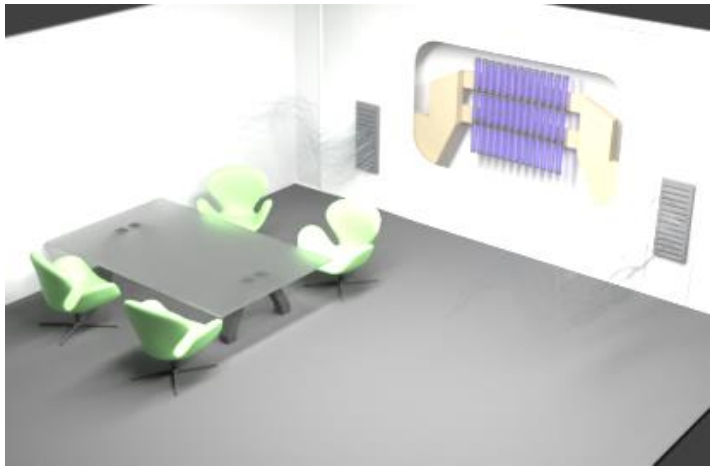


Possible and Planned Applications

- Storage of solar power in excited states for time shifted photoreaction



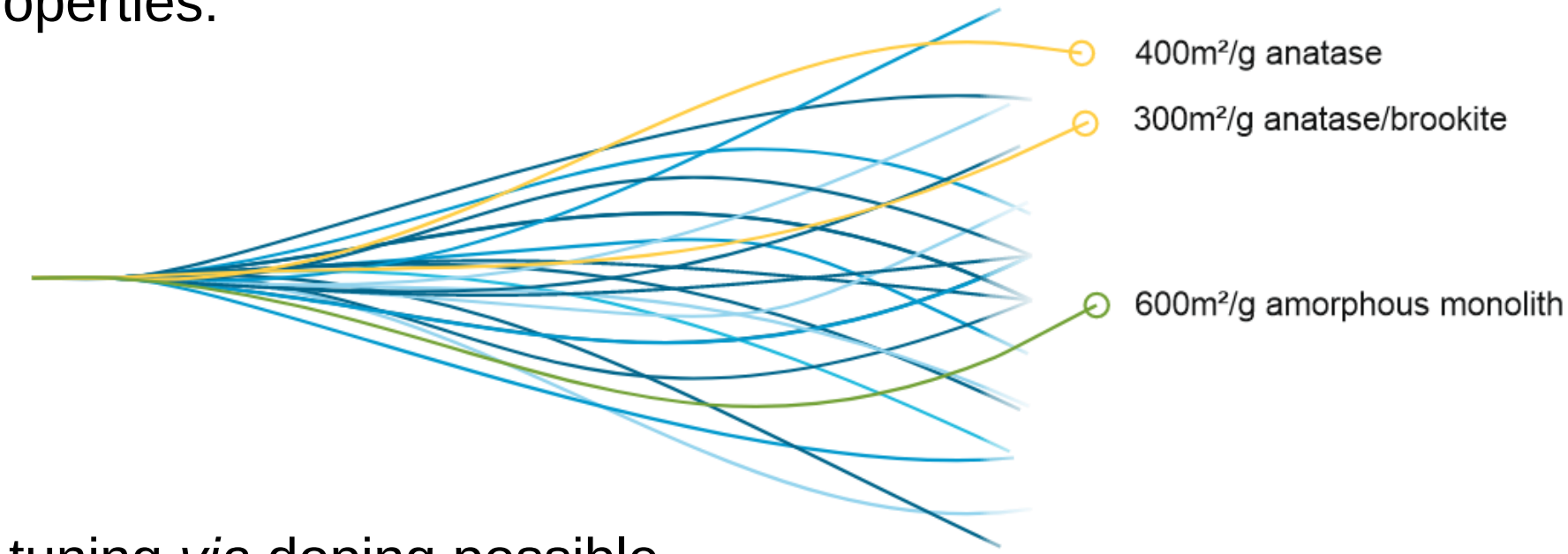
© Spartan Space



- Air conditioning and cleaning of capsuled compartments
  - Moon / Space habitat
  - Deep Sea

Conclusion and Outlook

- Titania aerogels can be synthesized with tunable properties:



- Band gap tuning *via* doping possible
- Properties of wet gels need to be further investigated
- Mechanical properties are being optimized

Thank you for your attention!

Topic: **Aerogels and How To Tailor Them for Photocatalysis**

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Authors: *P. Kuschmitz*, A. Rose, B. Milow, P. Voepel

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DFG Deutsche Forschungsgemeinschaft

SPP 2370 Nitroconversion

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