Projekt B6

Multiskalensimulationen zur Aufklärung des Stofftransports durch Kunststoffe mit PECVD-Beschichtung

16.04.2021

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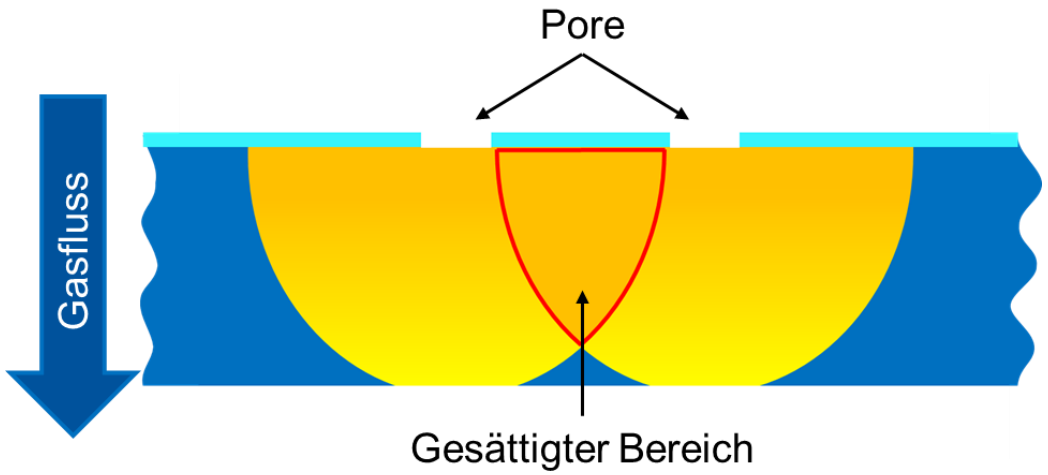
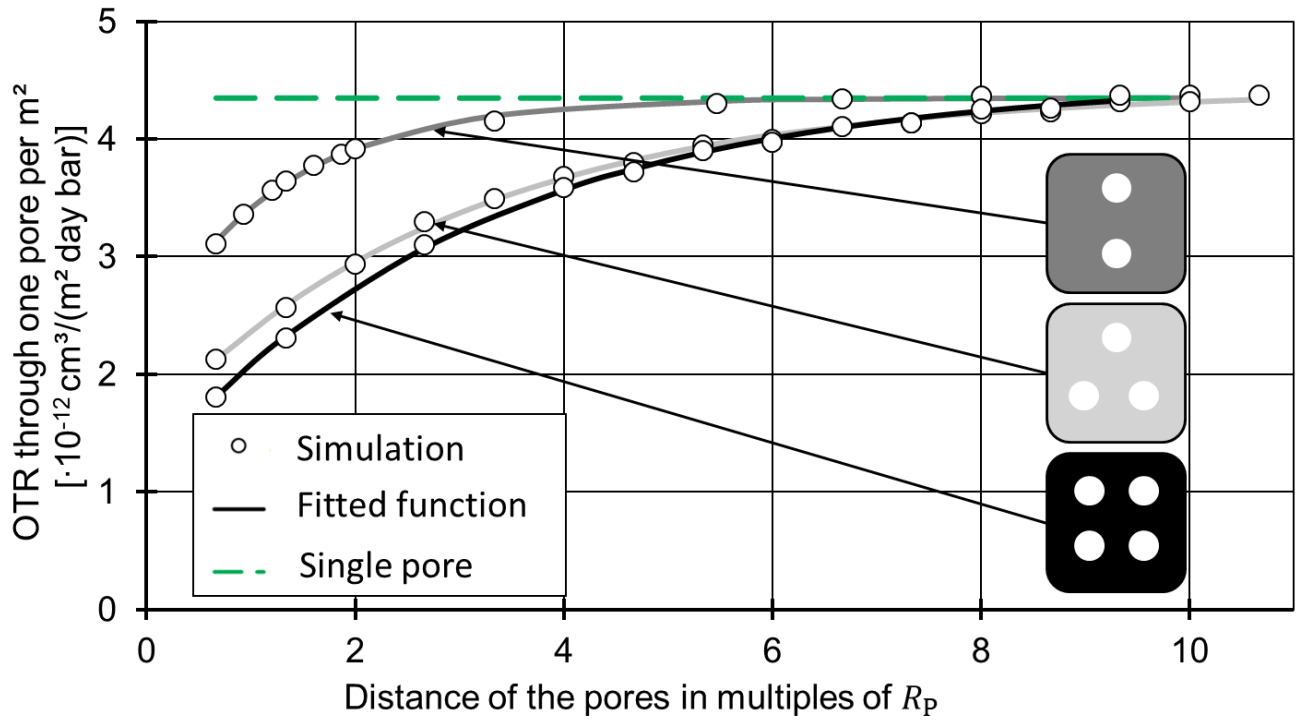
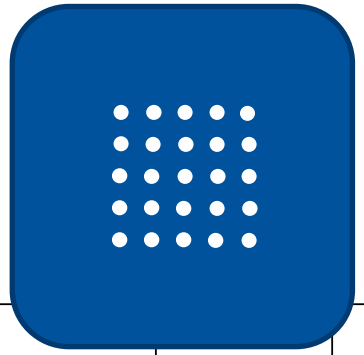
Beeinflussung benachbarter Poren // Simulation



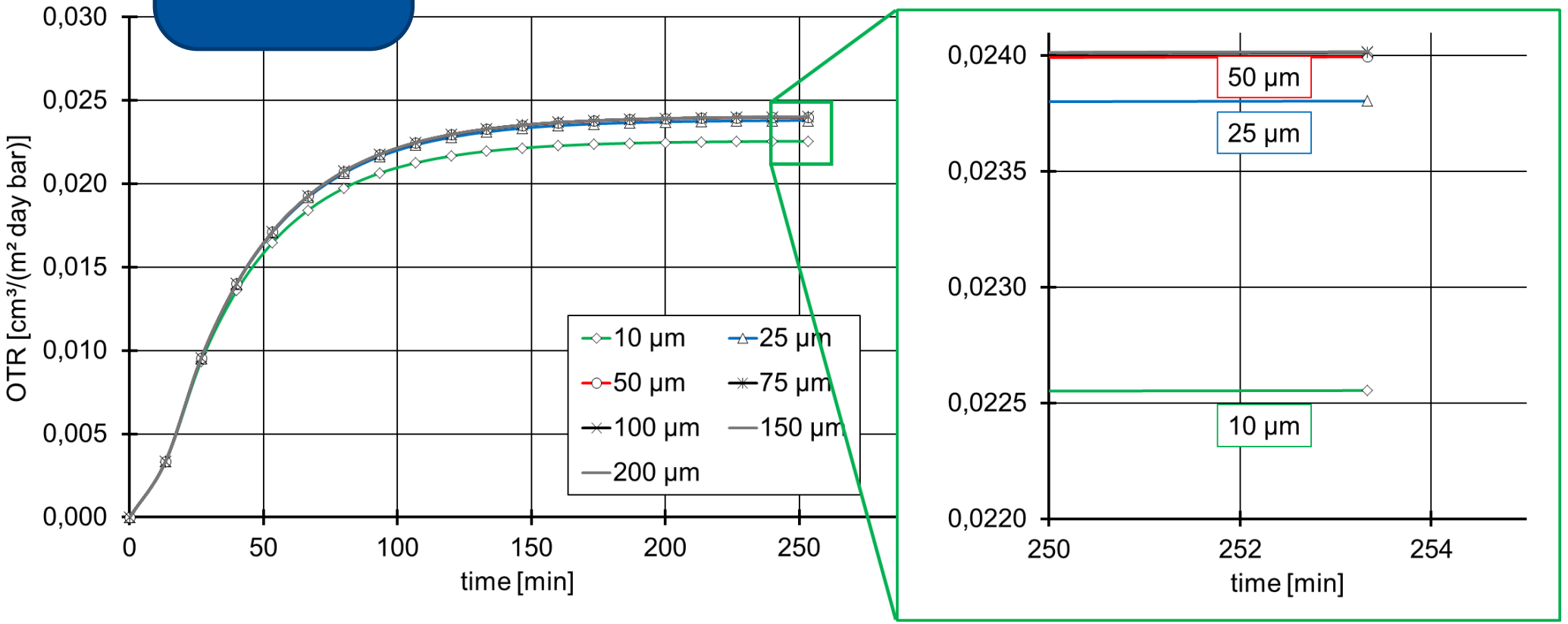
Porenpaare 2 , 3 und 4



Beeinflussung benachbarter Poren // Simulation



Porenraster 5 x 5 Poren



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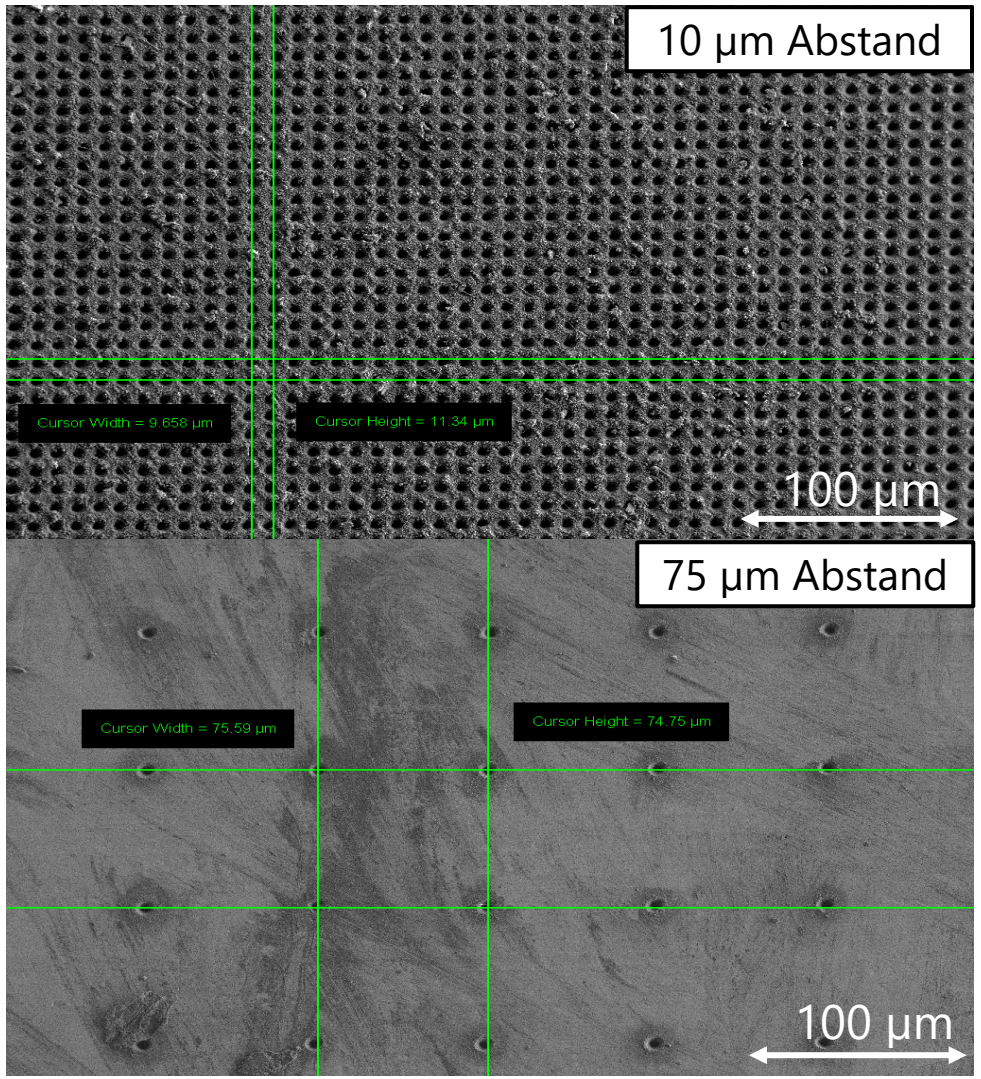
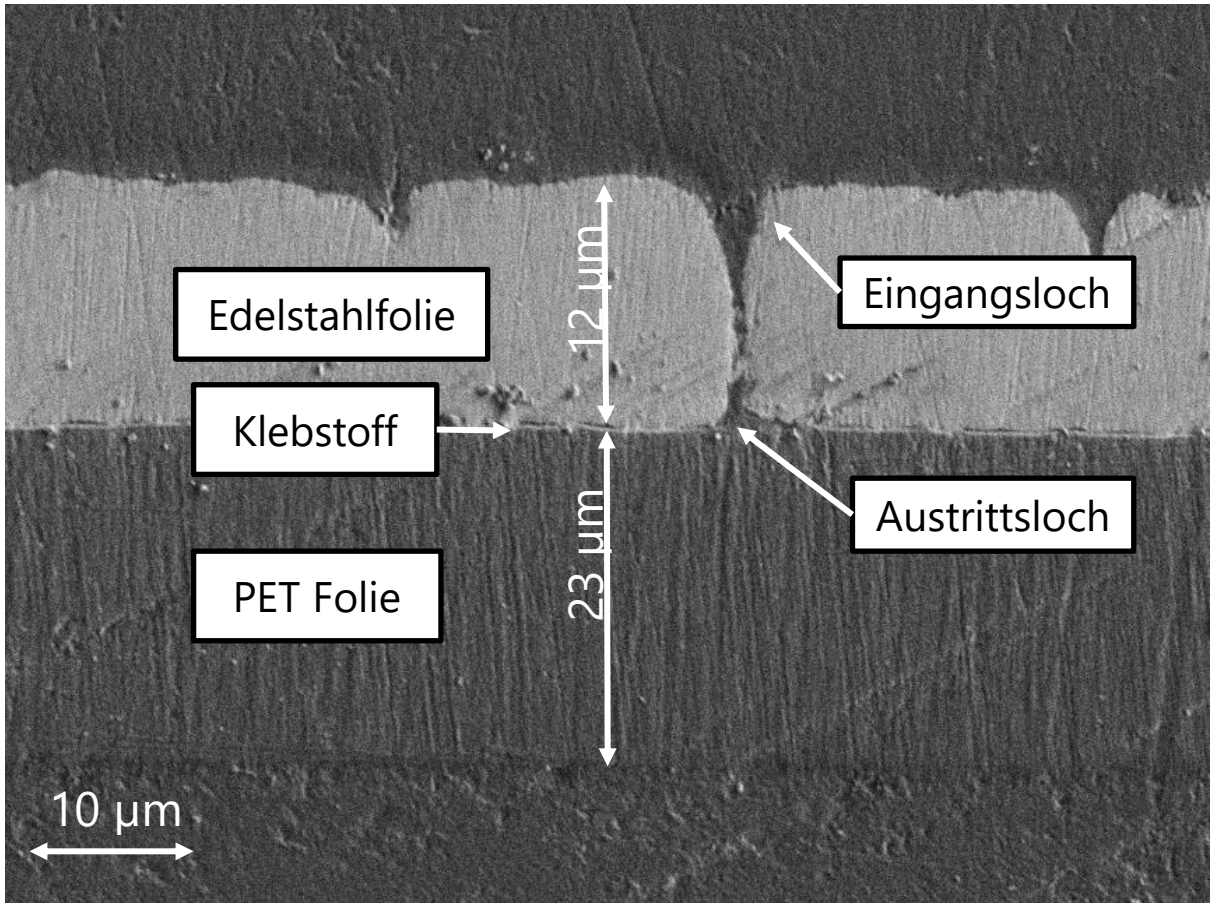
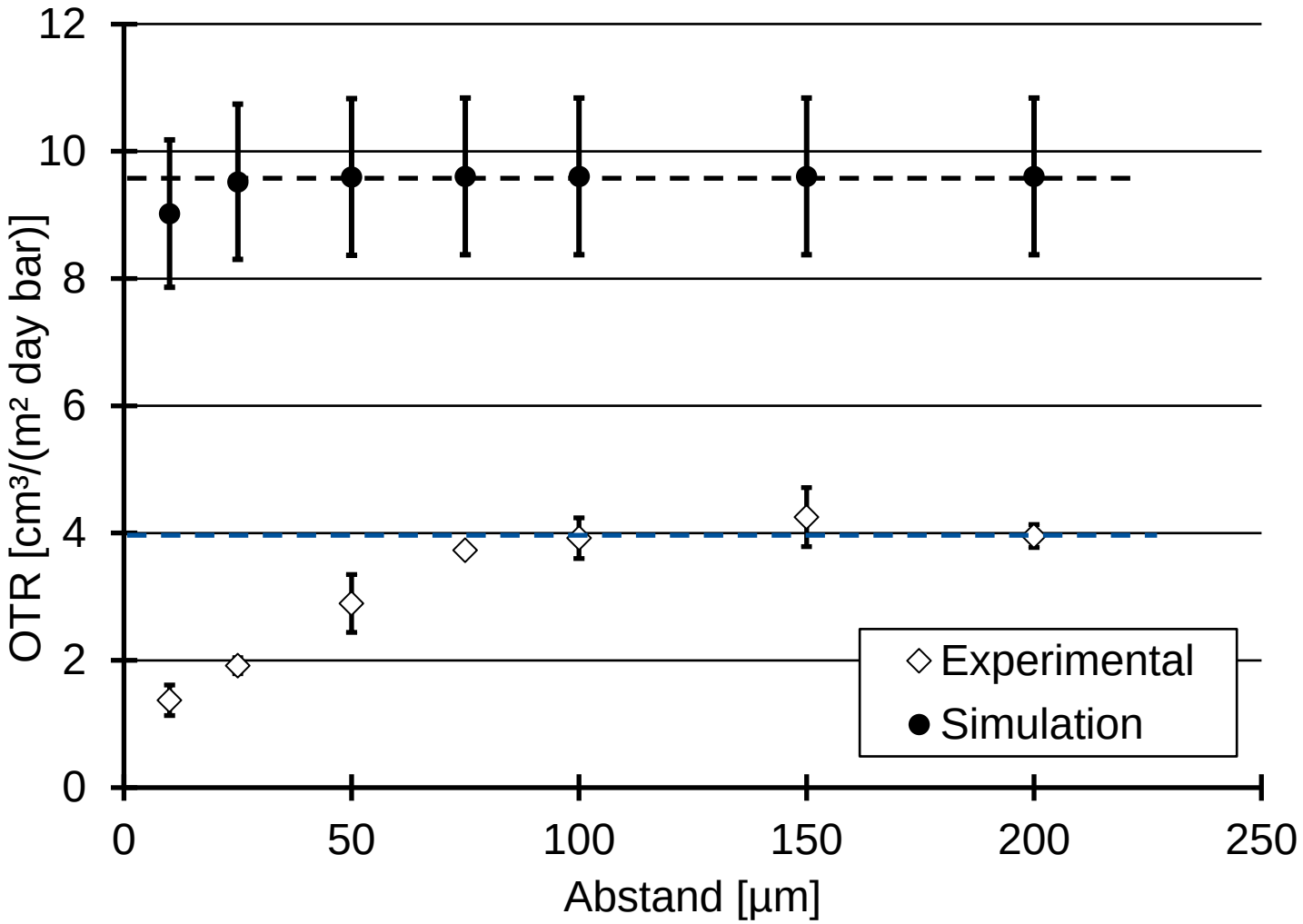
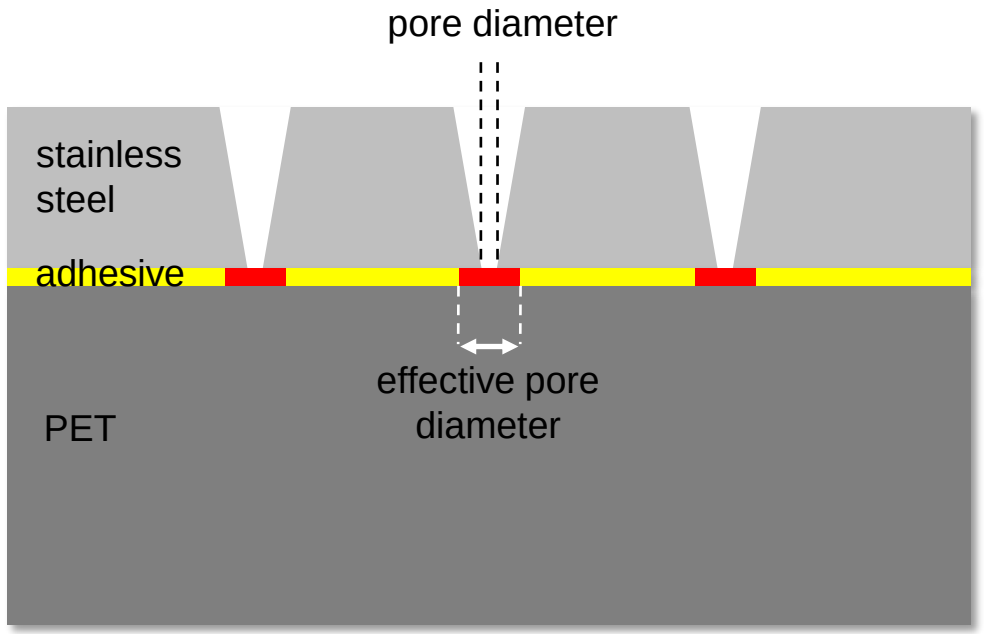
Beeinflussung benachbarter Poren // Experimentell





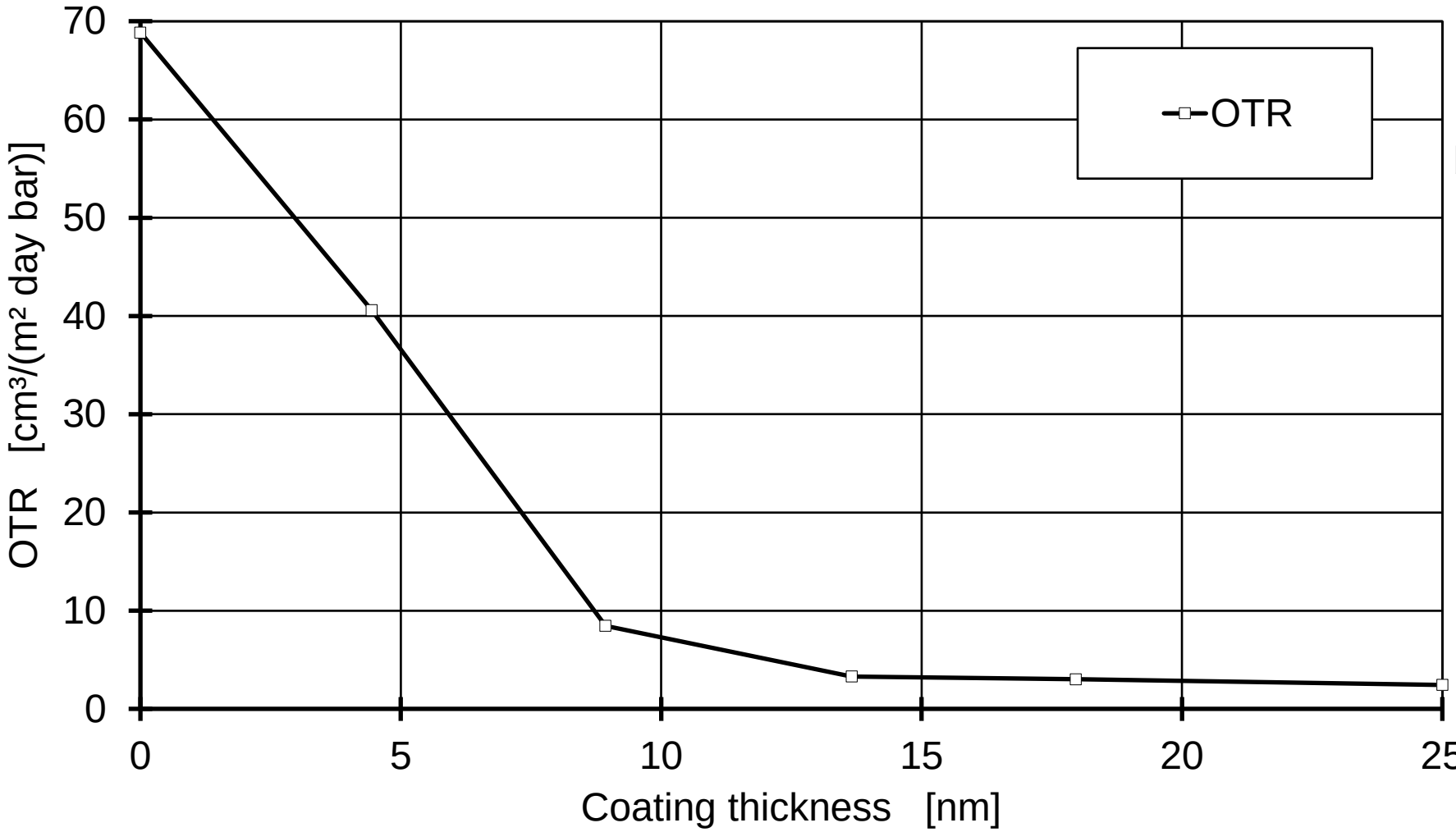
Beeinflussung benachbarter Poren // Vergleich Simulation und Experiment

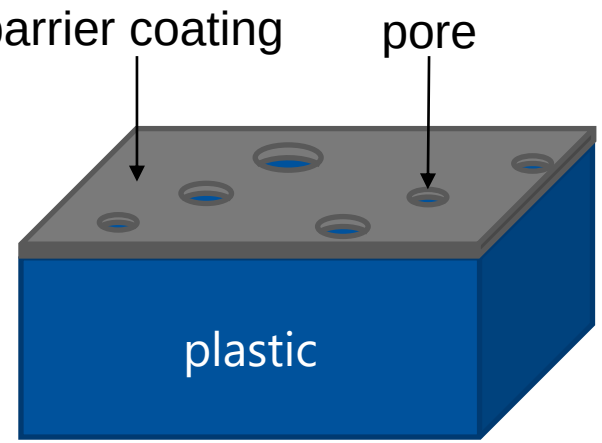




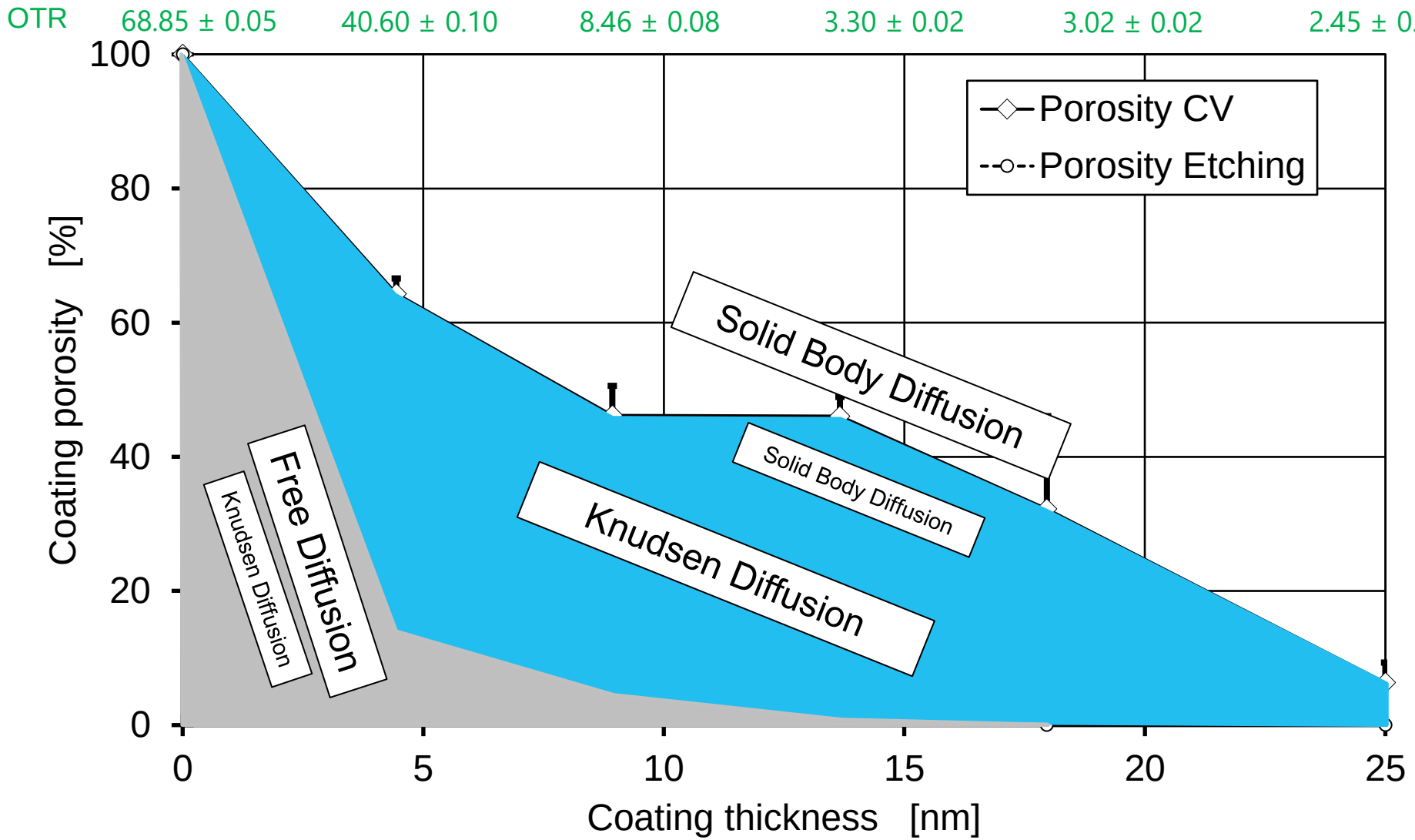
* Wilski 2021 *Influence of pore spacing in barrier coatings on the mass transport through plastics - a simulative and experimental approach, Thin Solid Films (eingereicht 01.2021)*

Diffusionsmechanismen durch porenbehaftete Barriereschichten (0s = unbeschichtete Referenz)





Diffusionsmechanismen durch porenbehaftete Barriereschichten (0s = unbeschichtete Referenz)



Dominating Diffusion Processes

Free + Knudsen Diffusion

d_P > 50 nm

Knudsen + Solid Body Diffusion

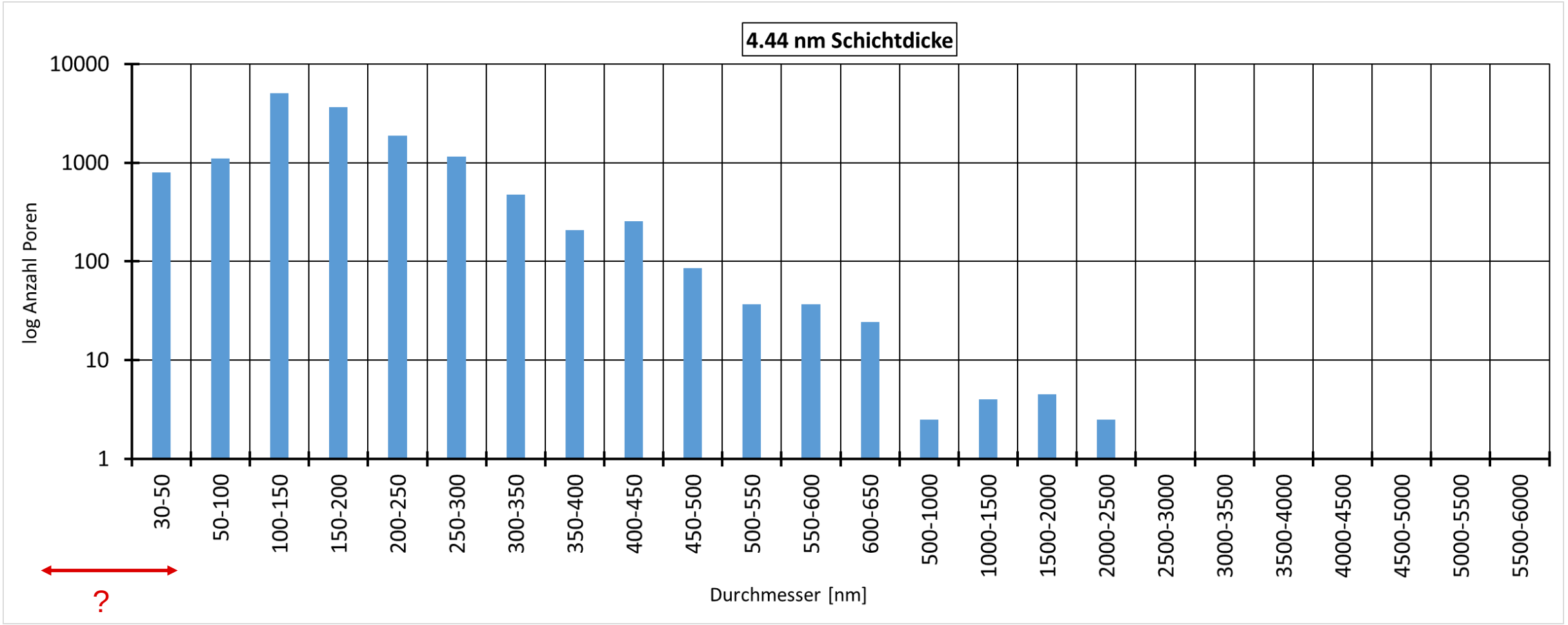
50 nm > d_P > 1 nm

Solid Body Diffsuion

d_P < 1 nm

S. Wilski et al. 2020 *Quantification of dominant diffusion processes through PECVD-coated plastics by combining two complementary methods for porosity analysis. JPhysD. 04/2020*

Diffusionsmechanismen durch porenbehaftete Barriereschichten
Porenauswertung



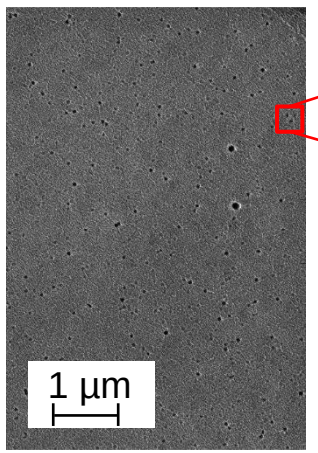
Wilski, Zysk: Multiscale Simulations of Oxygen through barrier Coatings (in Bearbeitung, 05.2021)

Porenauswertung
Fehlerquellen der digitalen Bildverarbeitung

Originalbild

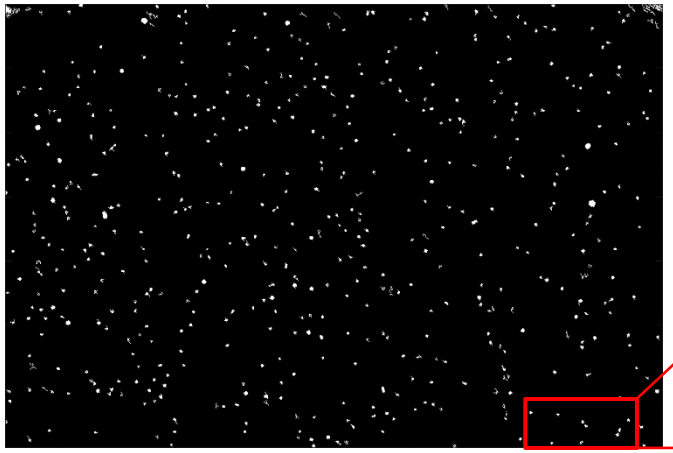
Binärbild

Filterbild



2 Defekte

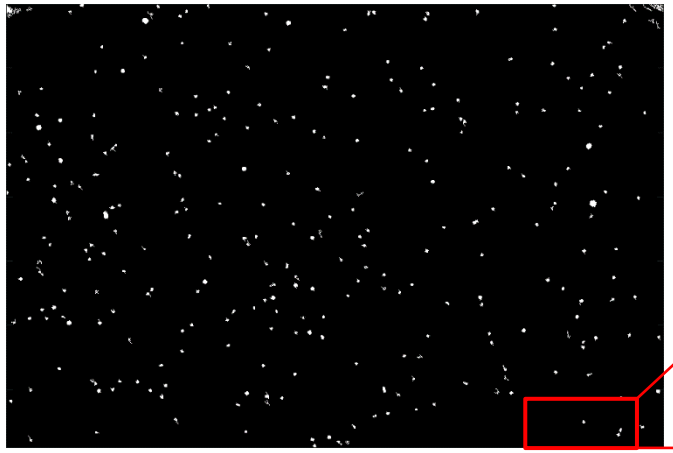
3 Defekte Threshold 1.0



Filter 11 9 Defekte

3 Defekte

Threshold 0.95



3 Defekte

Filter 16

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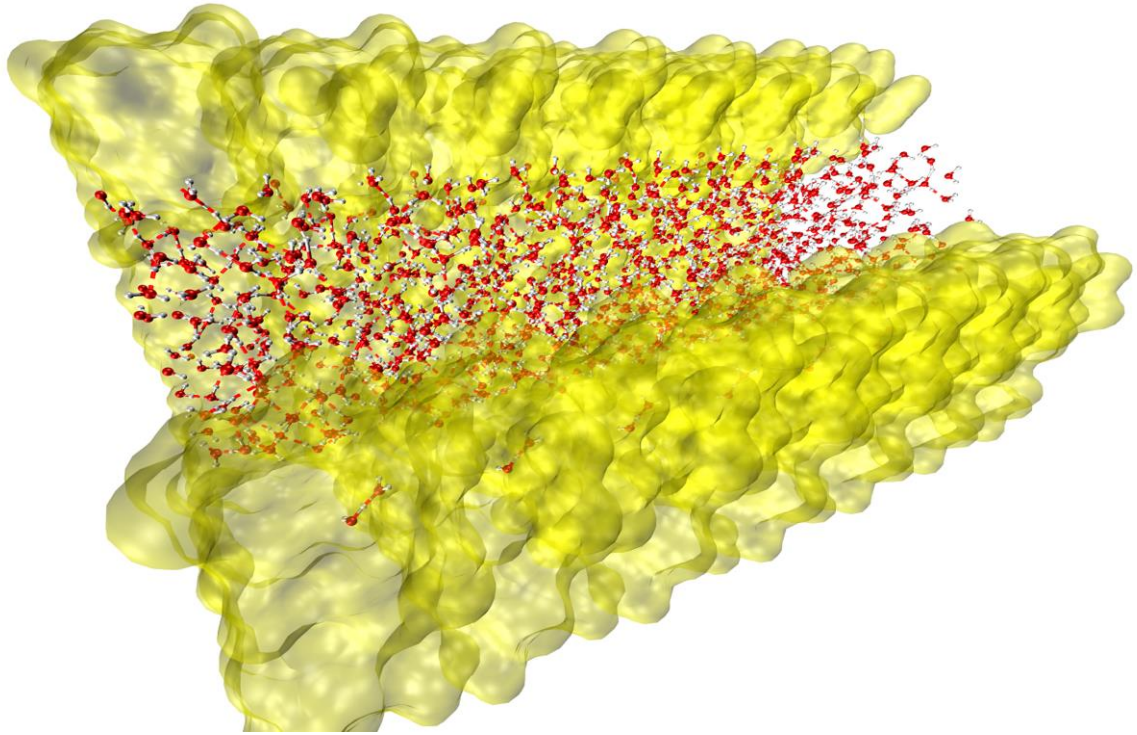
Silica Pore Structure and Dynamics

Computational Details

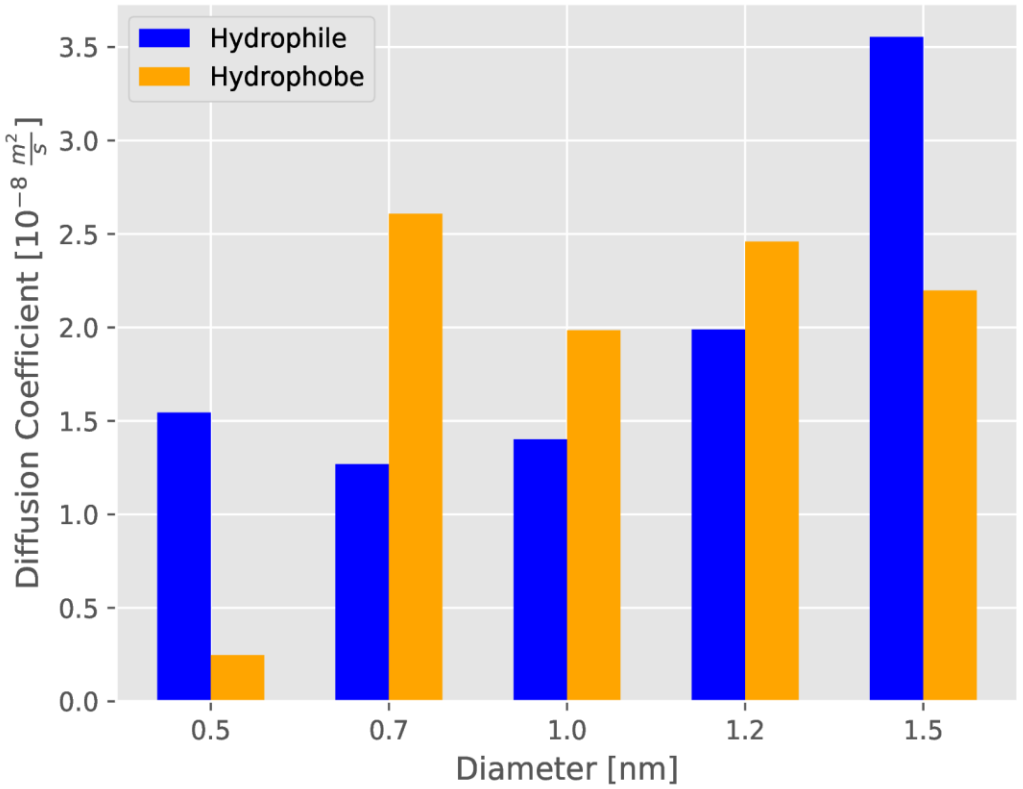
- Silica pores with diameters from 0.5 to 1.8 nm
- Hydrophilic Functionalization (OH)
- Hydrophobic Functionalization (CF3)
- Water and oxygen vapor as medium
- Semi-empirical MD Method

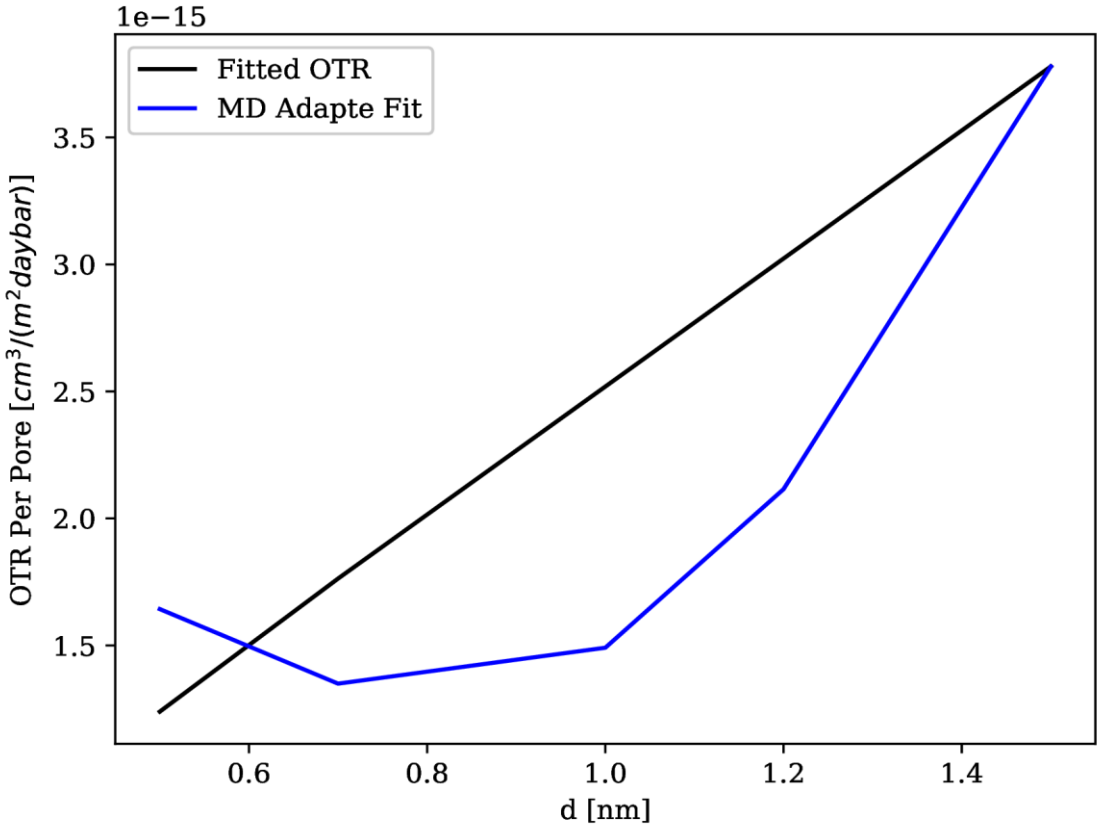


Overall Results

- Large pores inhibit bulk properties, smaller pores show lower Diffusion
- Generally faster Diffusion in hydrophobic pores
- Change in Water structure/orientation responsible for Diffusion

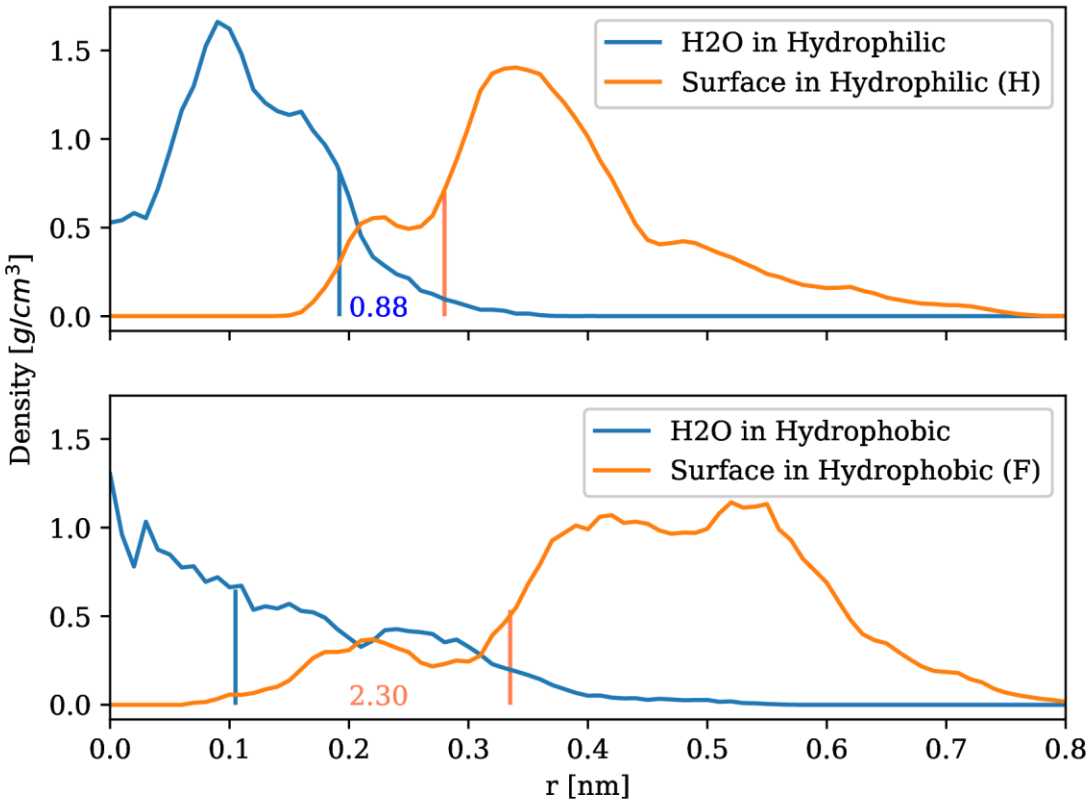
Oxygen Vapor Dynamics

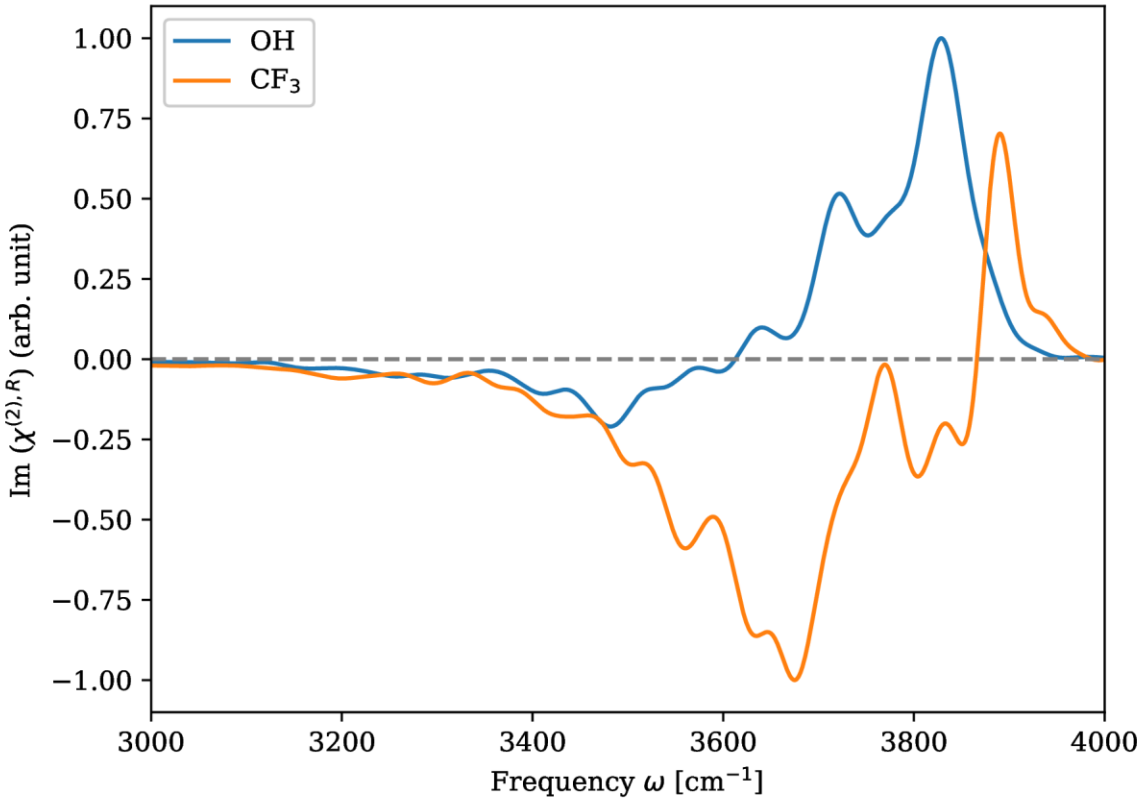




(B6 IKV+UPB) Wilski, Zysk: *Multiscale Simulations of Oxygen through barrier Coatings* (Q2, 2021)

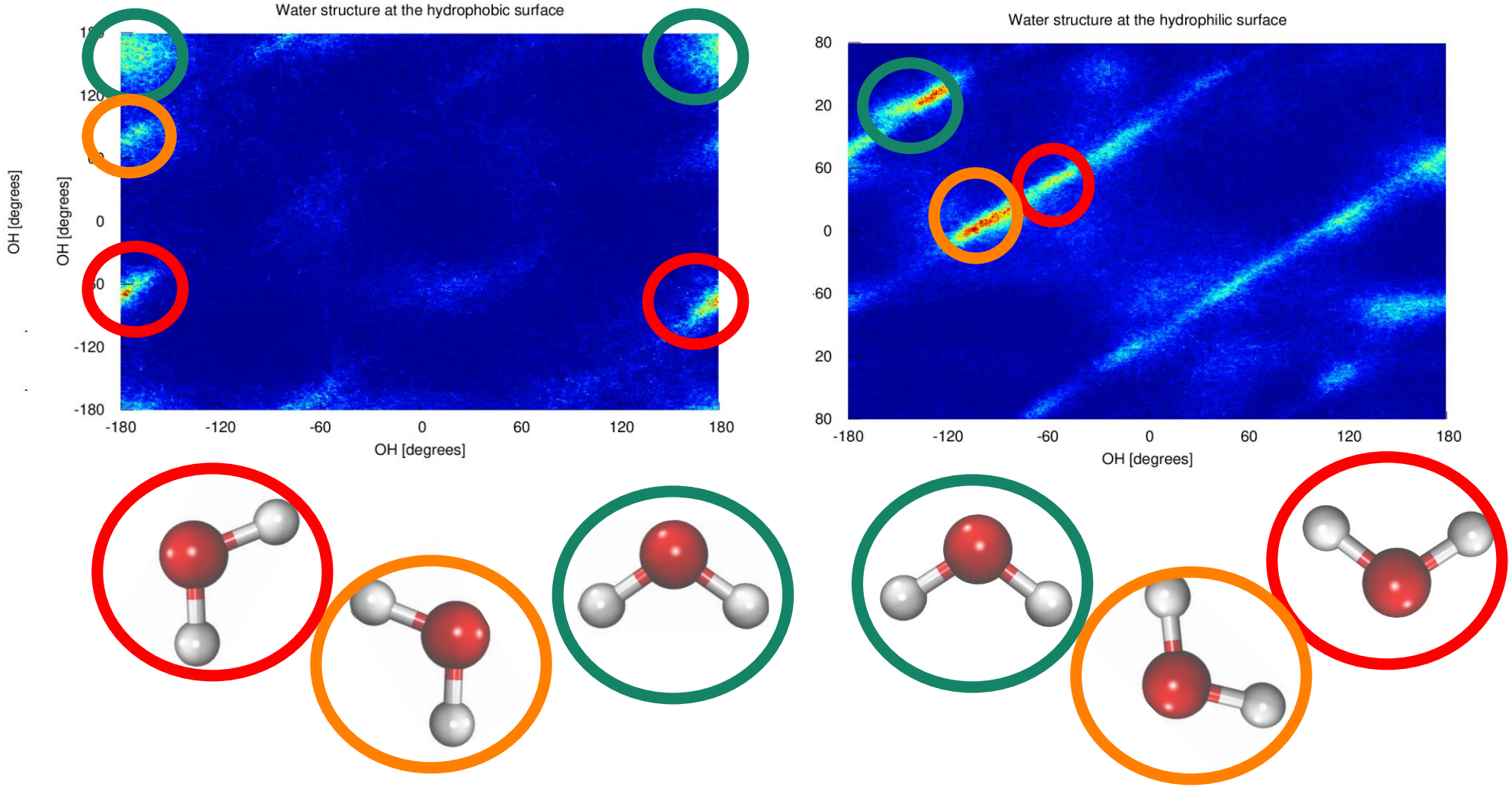
Water Structure at the Pore Surface





(B6 UPB) F. Zysk et al 2021 *Impact of hydropathy on the structure and dynamics inside SiO2 nanopores* (Q2, 2021)

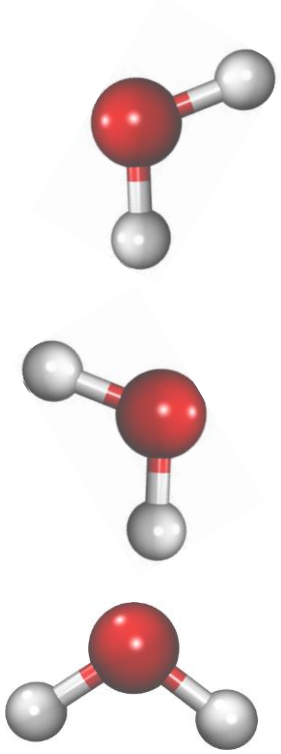
H2O Orientation Analysis

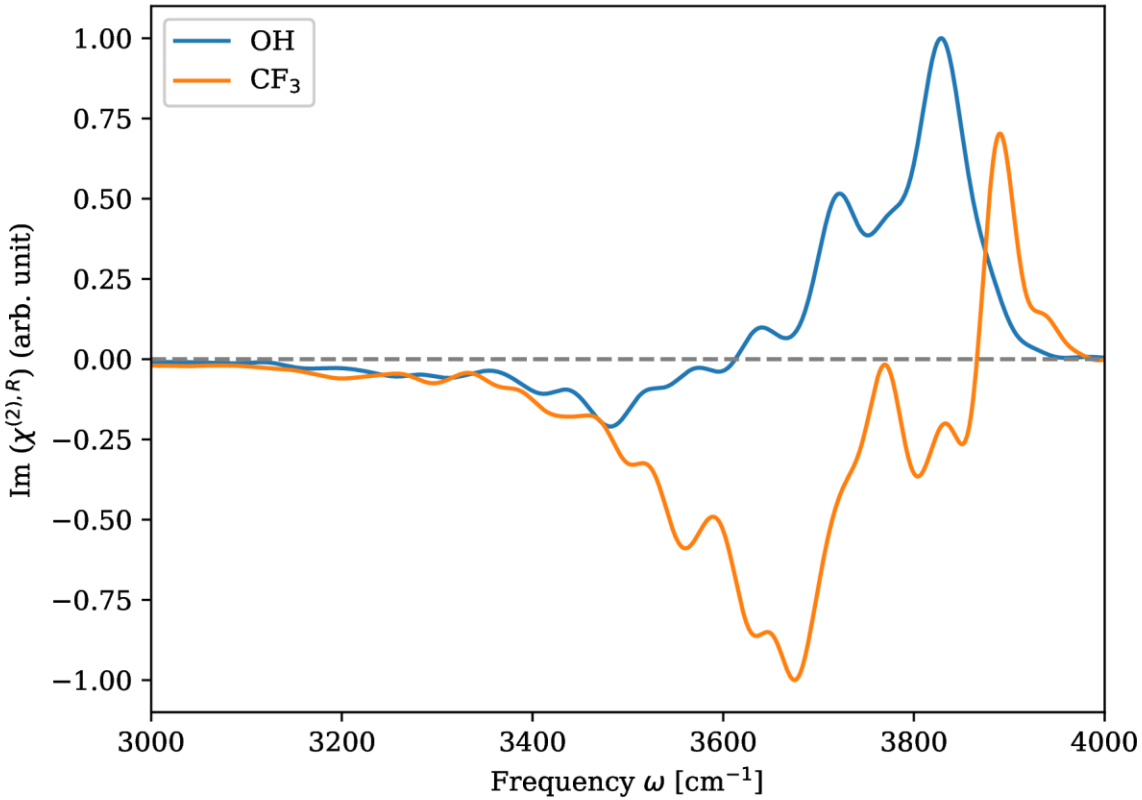


(B6 UPB) F. Zysk et al 2021 *Impact of hydropathy on the structure and dynamics inside SiO2 nanopores* (Q2, 2021)

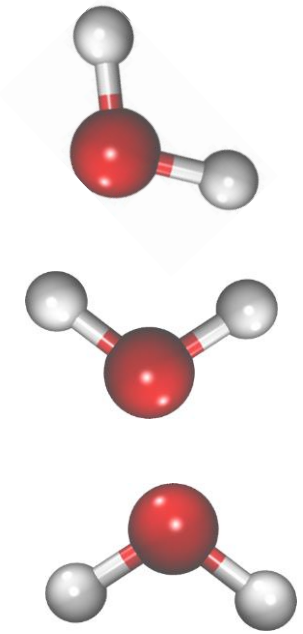
Water Structure at the Pore Surface

Hydrophobic (CF3)



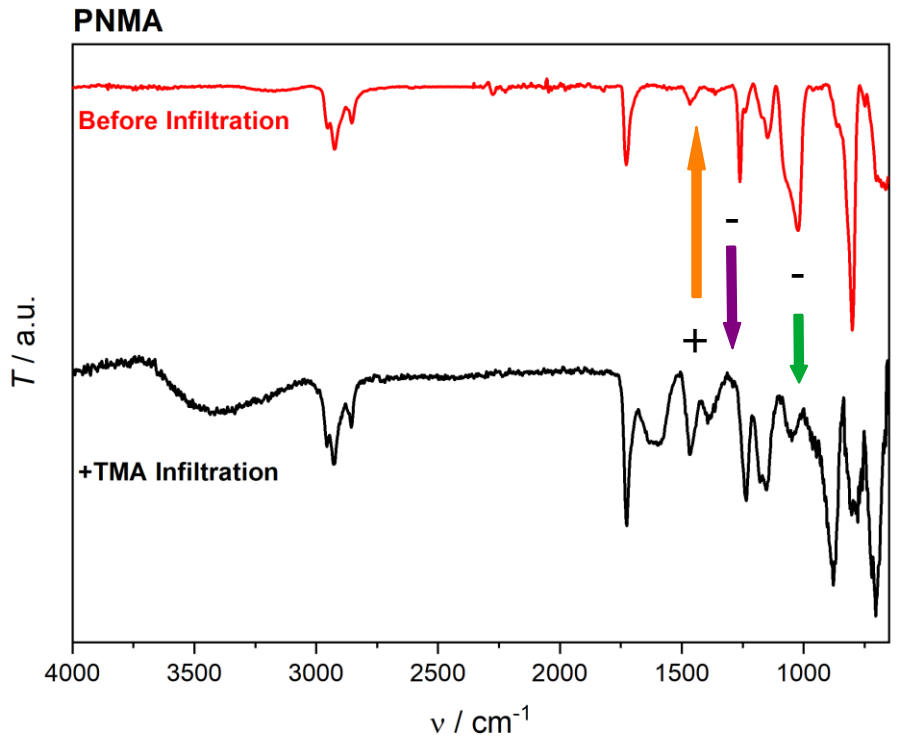


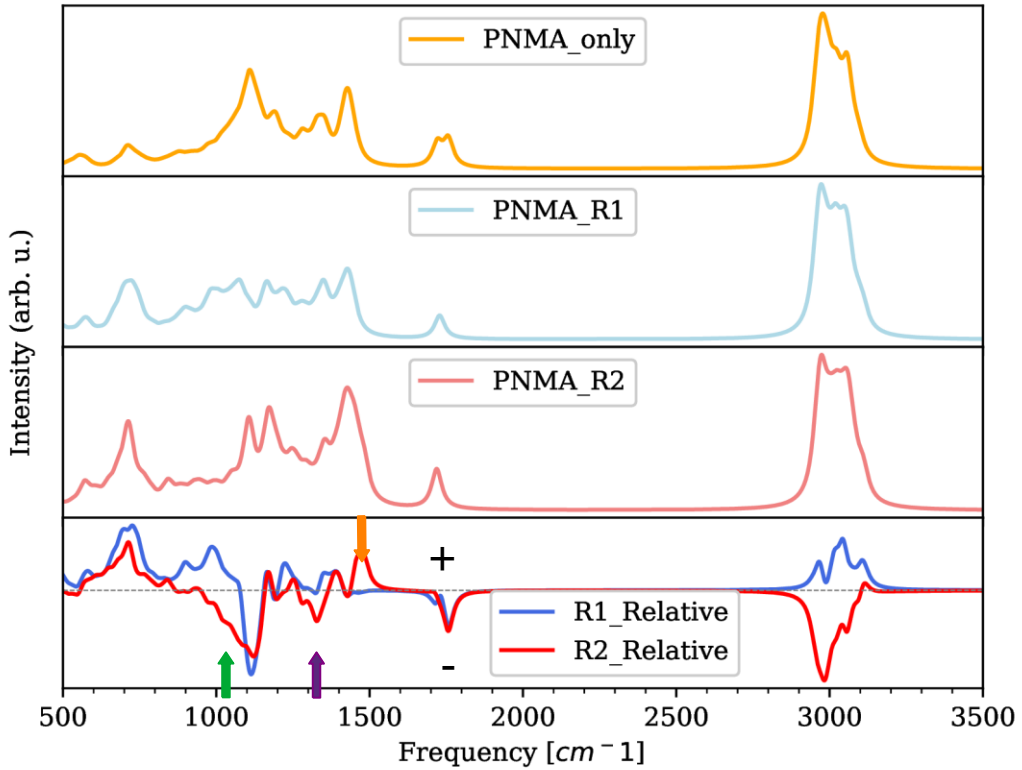
Hydrophilic (OH)



(B6 UPB) F. Zysk et al 2021 *Impact of hydropathy on the structure and dynamics inside SiO2 nanopores* (Q2, 2021)

TMA Vapor Infiltration into Polymers





Energy R2-R1: -1.036 eV

IR indicates R2 very dominant

Energy and IR favor R2 strongly

(B4/UPB) L. Mai, F. Zysk *VPI of TMA into polyesters: Experimental ALD type approach complemented by theoretical investigations*

Veröffentlichungen

- **Veröffentlicht:**
  - (IKV) S. Wilski et al. 2020 *Quantification of dominant diffusion processes through PECVD-coated plastics by combining two complementary methods for porosity analysis. JPhysD. 04/2020*
  - (UPB) N. K. Kaliannan et al 2019 *Impact of intermolecular vibrational coupling effects on the sum-frequency generation spectra of the water/air interface*, *Molecular Physics, 1-10 05/2019*
- **Eingereicht:**
  - (B6 IKV) Wilski 2021 *Influence of pore spacing in barrier coatings on the mass transport through plastics - a simulative and experimental approach, Thin Solid Films (eingereicht 01.2021)*
  - (B7/UPB) How is carbon dioxide transported through humidified facilitated transport membranes - experimental analysis coupled with molecular dynamic simulations, J of Membrane Science
- **In Bearbeitung:**
  - B6 IKV+UPB Wilski, Zysk: Multiscale Simulations of Oxygen through barrier Coatings (in Bearbeitung, 05.2021)
  - (B6 UPB) F. Zysk et al 2020 *Impact of hydropathy on the structure and dynamics inside SiO2 nanopores* (Q2, 2021)
  - (B4 +B6/UPB) L. Mai, F. Zysk *VPI of TMA into polyesters: Experimental ALD type approach complemented by theoretical investigations*

Appendix