



We create chemistry

# Artificial Intelligence in Materials Research

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Digitalization in R&D

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PUBLIC



# Content

## Advanced Materials

### Vision

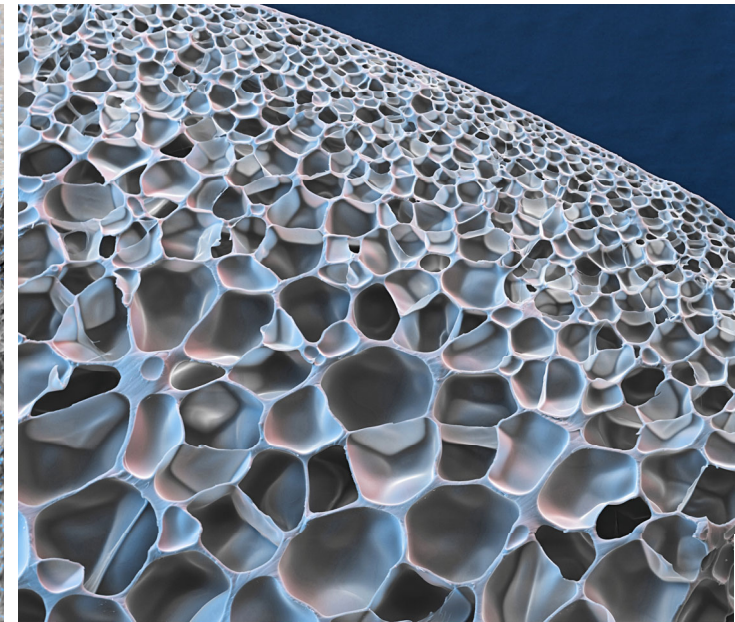
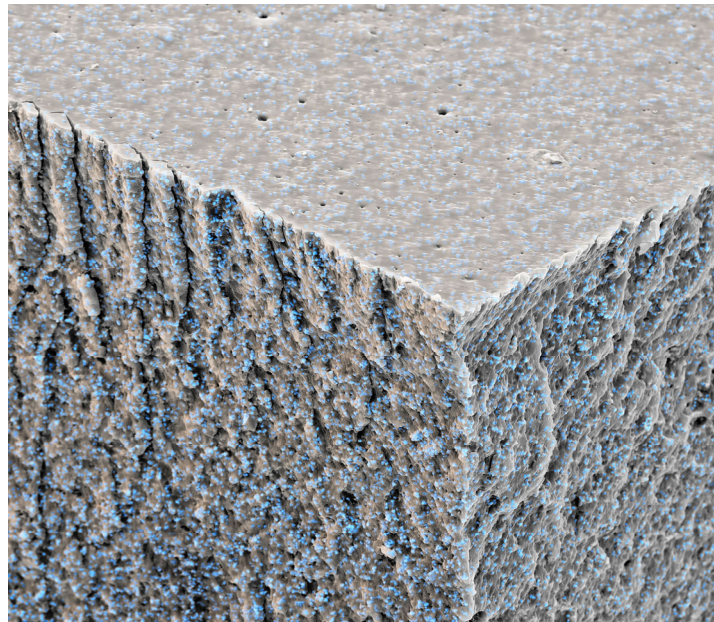
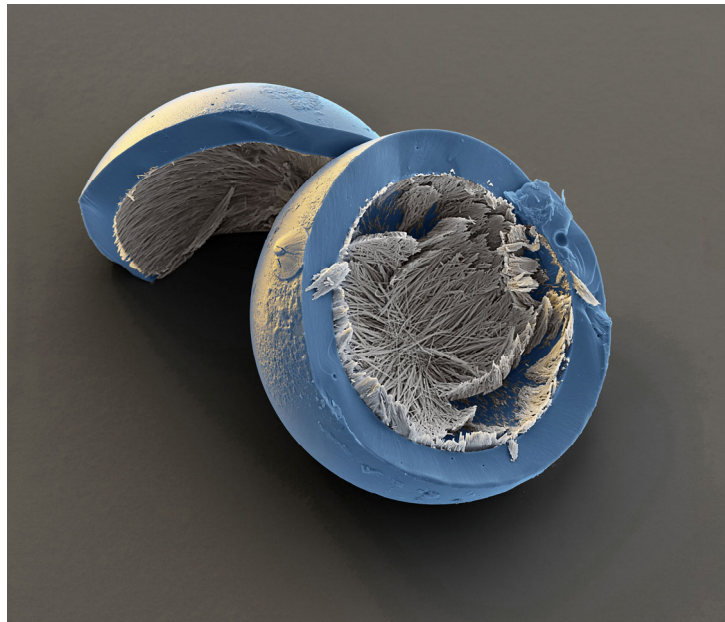
### Challenges

### Example

## Supercomputing

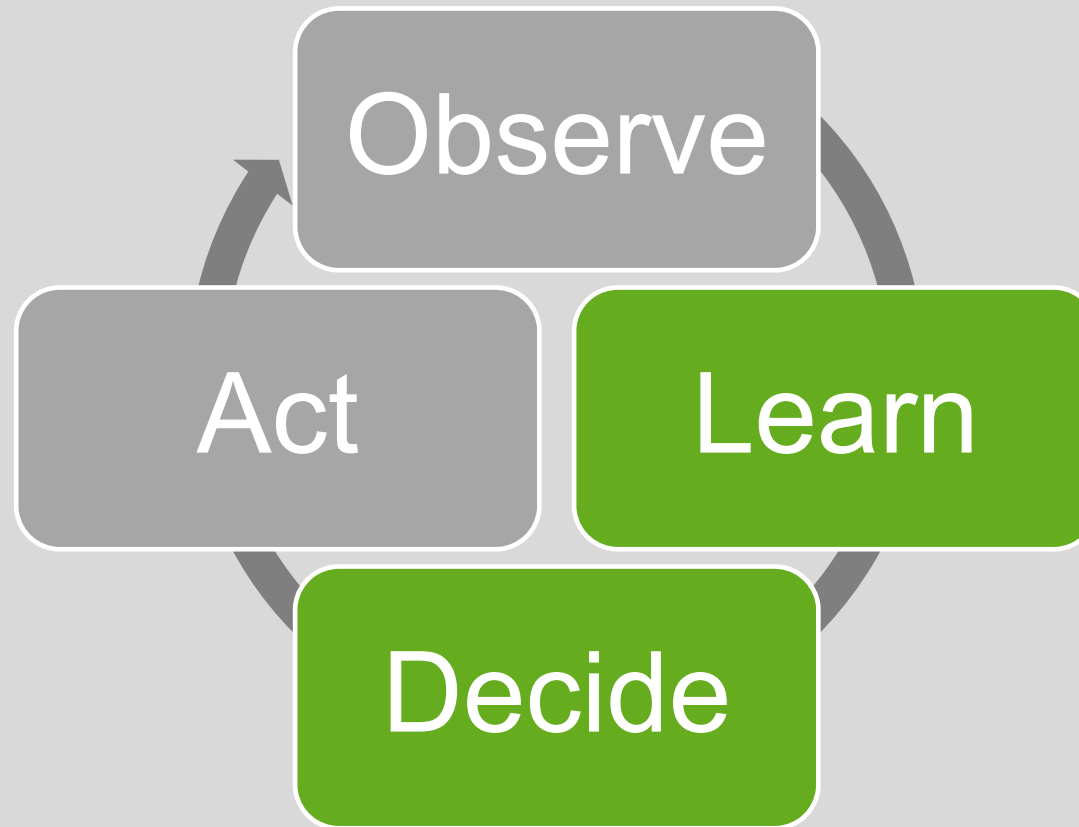
# Advanced Materials

# Advanced Materials



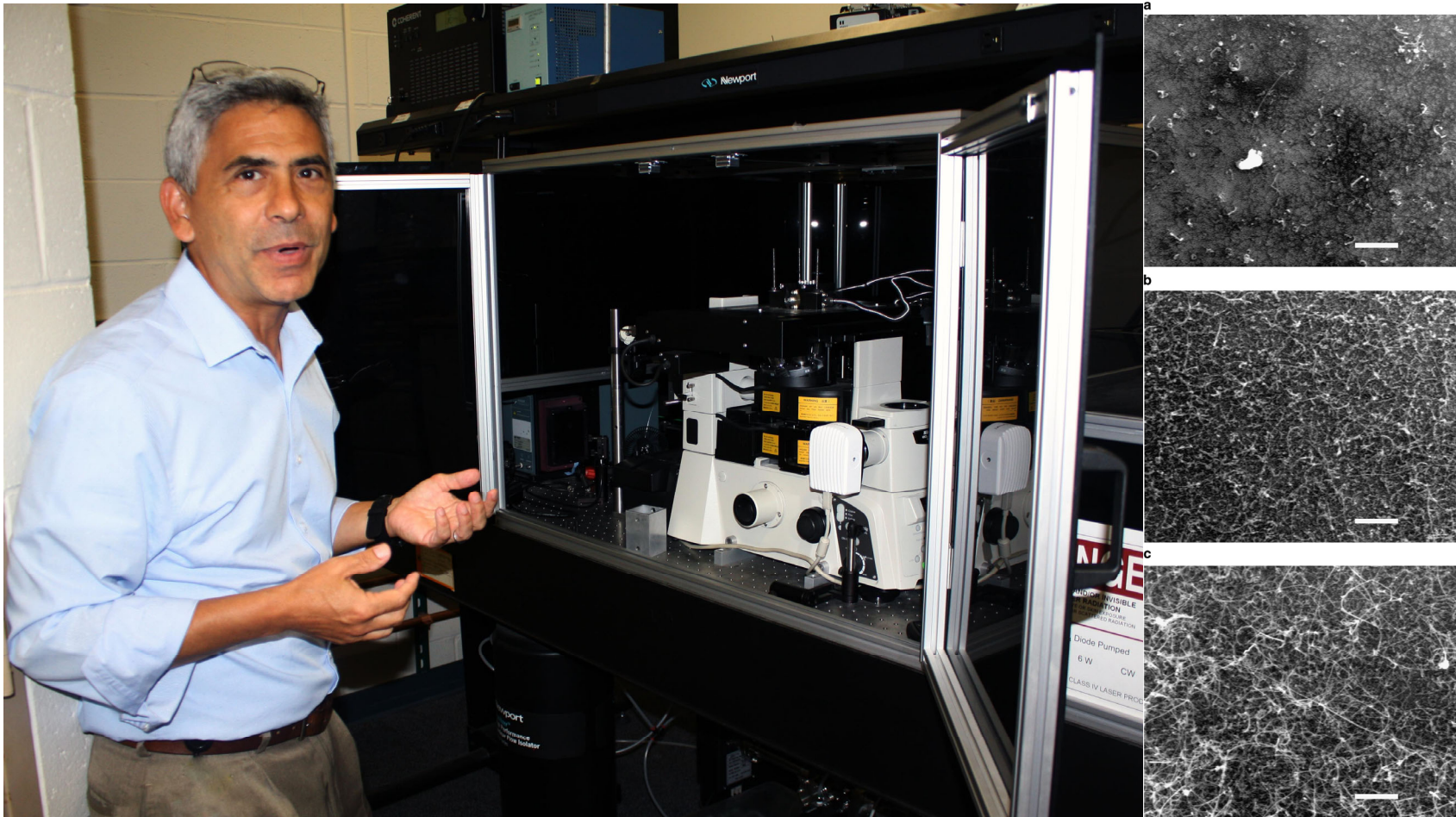
# Vision

# Artificial Intelligence System



# „Autonomous Research System“

presented by Nikolaev et al. from Air Force Research Lab published in npj Computational Materials, 2016



# Challenges



# Product Research & Development in Material Science



Material Composition & Process Conditions

$x$



Unknown Response

$f(x)$

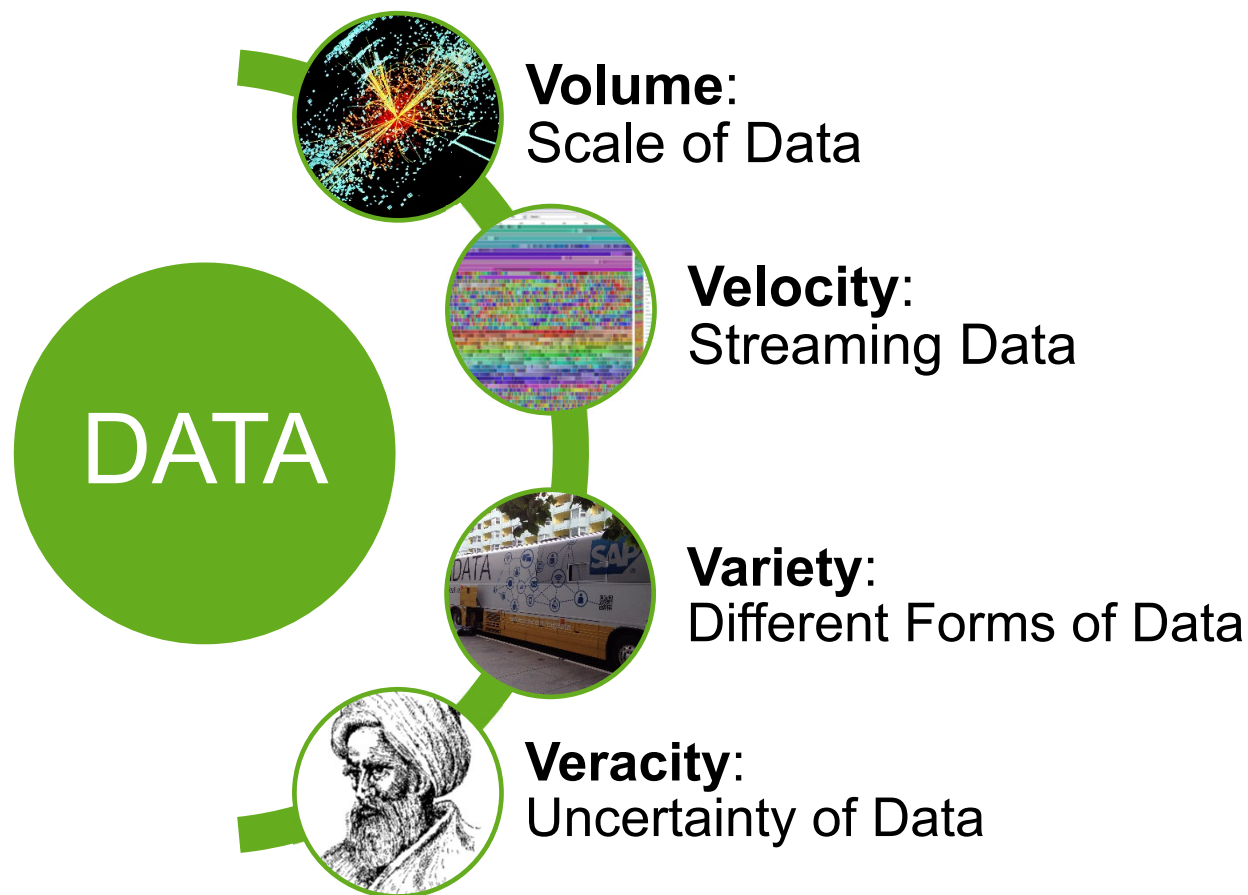


Desired Material Property

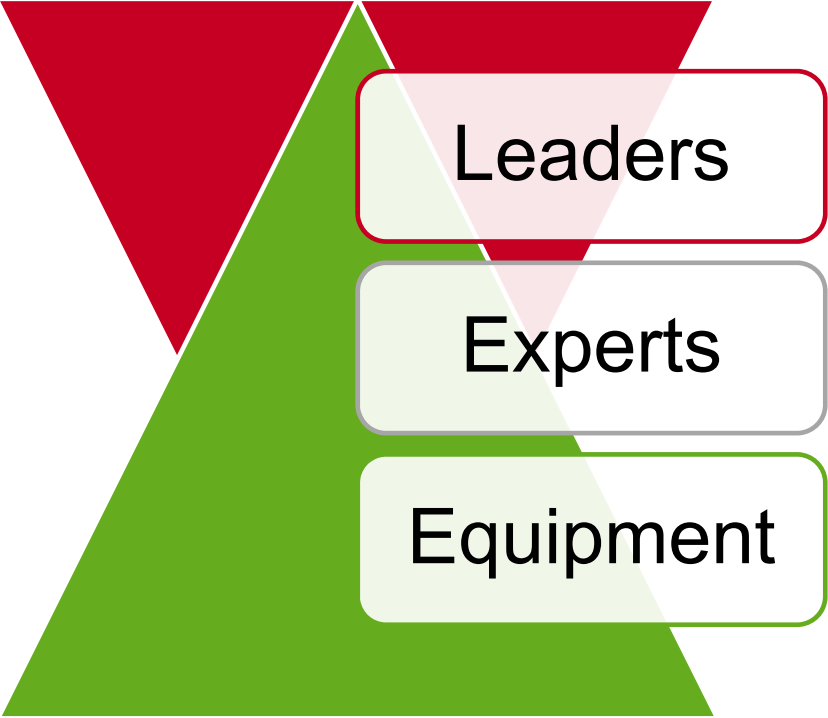
$\arg \min f(x)$

efficient & generic procedure to optimize an unknown complicated objective that is expensive & noise to evaluate?

# Challenge: Learning



# Challenge: Decisions



„Stat. Consult.“

„ML Solution“

„AI System“

# Example

# New coating from scratch with empirical optimization

## [ Target

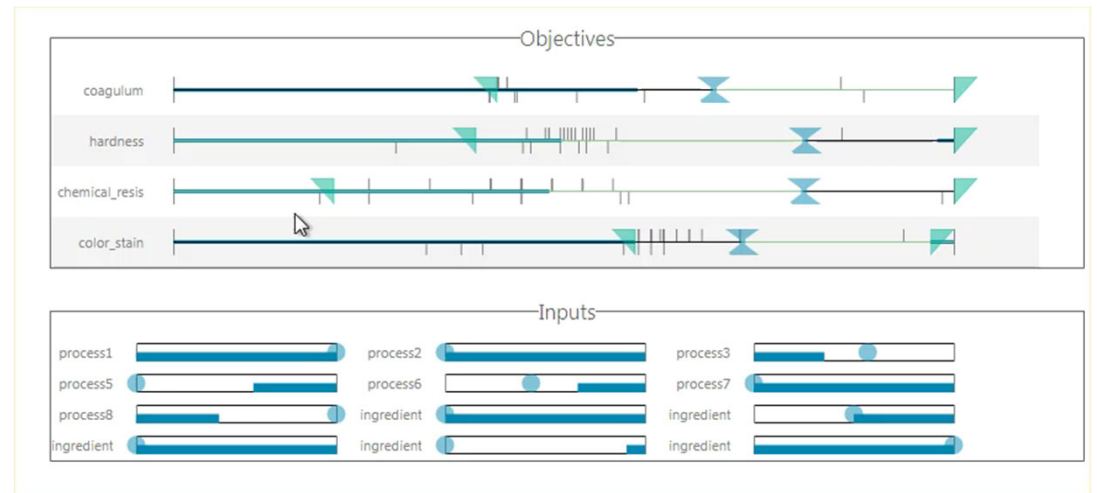
Develop novel water-based recipe with high aesthetic appearance on wood

## [ Challenge

No existing recipe as basis to quickly close portfolio gap

## [ Contribution

DoE followed by optimization provided a recipe after 3 months and the desired properties after 6 months



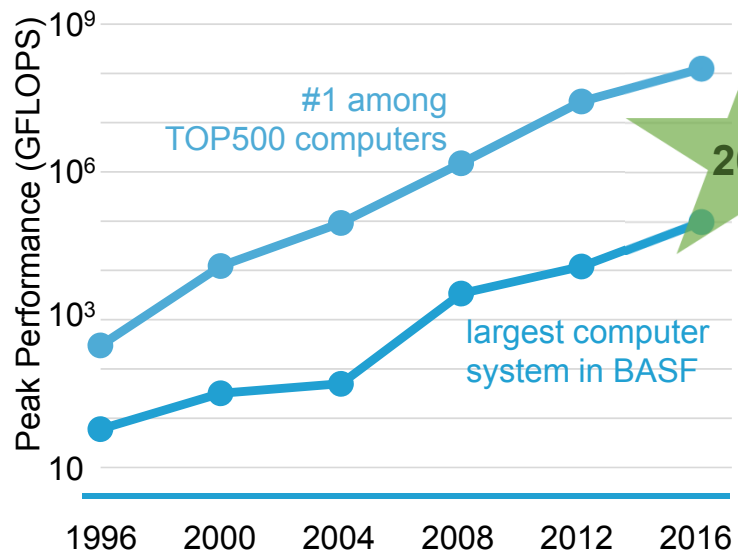
QRITERIA, co-developed by ITWM

**BASF**  
We create chemistry

# Supercomputing

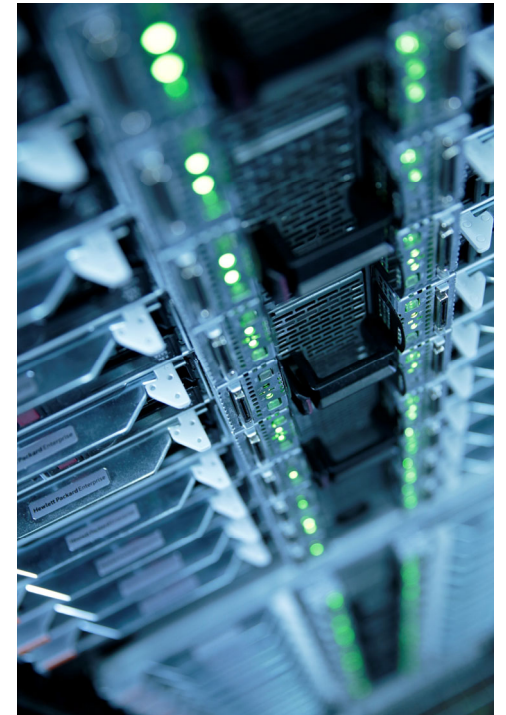
# Supercomputing at BASF

## BASF HPC history



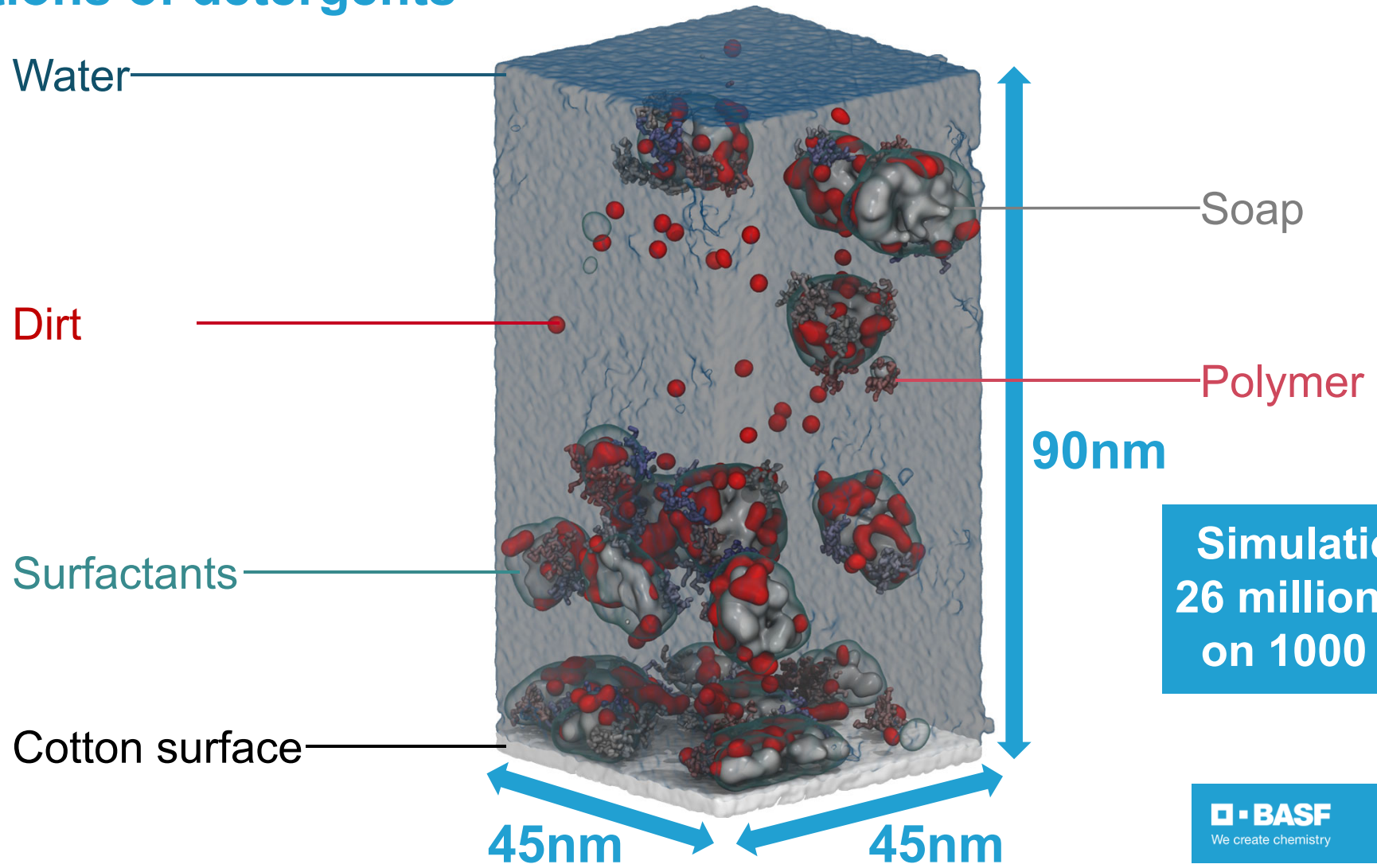
## Invest to shorten project timelines

- QURIOSITY significantly improves modeling
- Quantum Chemistry (100 → 1000 atoms) e.g. solvents, surfaces, solid states
- Soft matter (10,000 → 1,000,000 atoms) e.g. enzymes, thickeners, polymer solutions
- Full 3D models for CFD with multiphase flow
- Deep Learning



Significant opportunity for BASF to establish leadership in R&D supercomputing

# Simulations of detergents

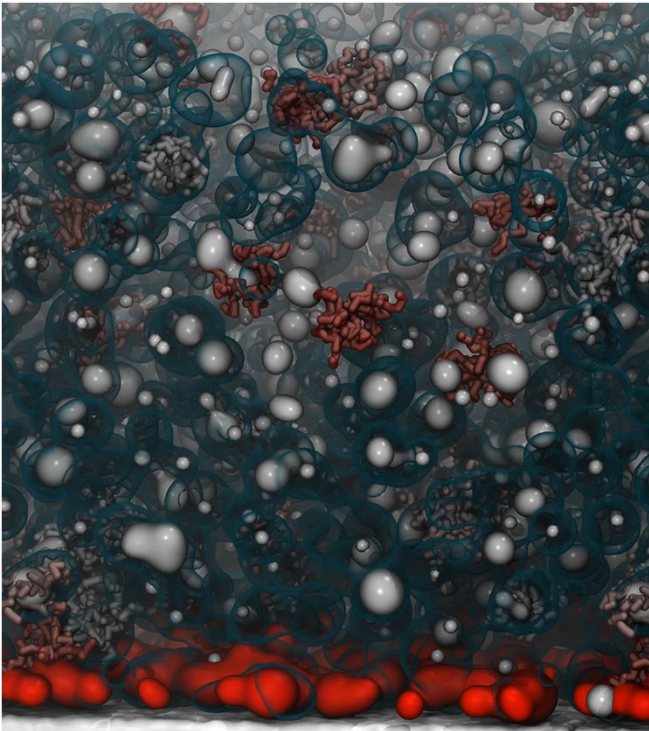
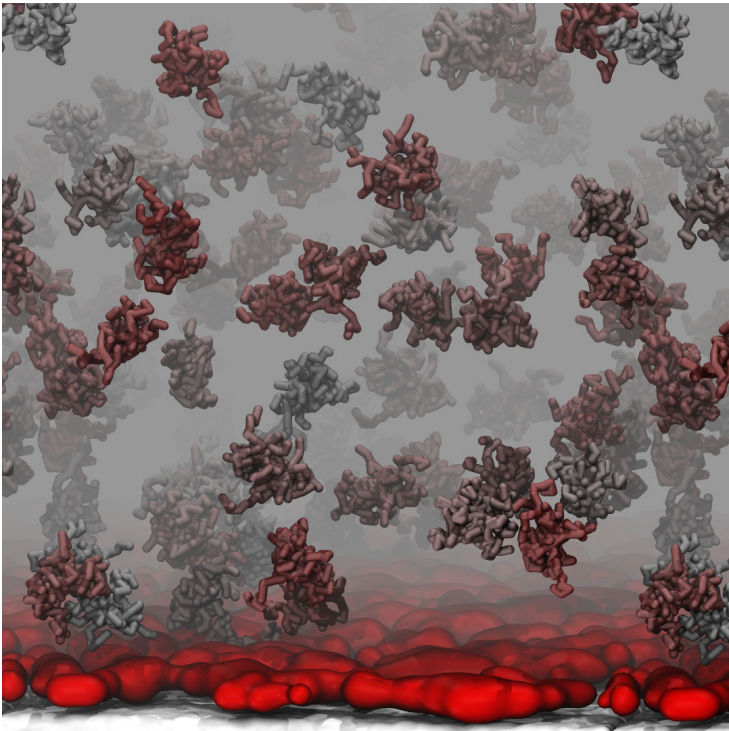


**Simulations of  
26 million atoms  
on 1000 cores**



# Cleaning polymer

Start



End

