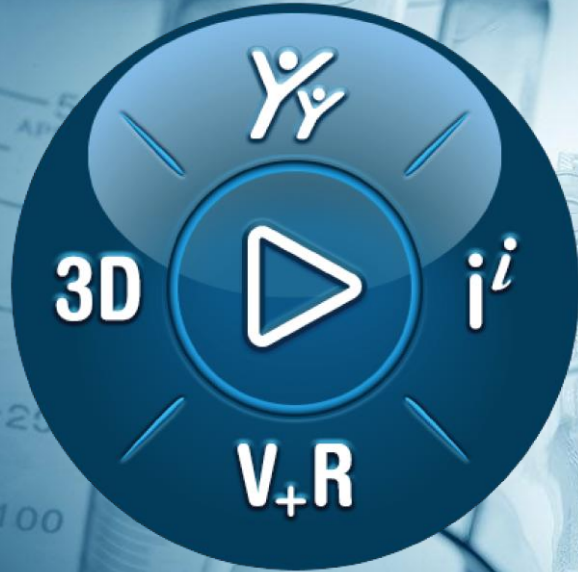


# DIGITAL TRANSFORMATION IN THE LAB DELIVERING EFFICIENCY & SUSTAINABILITY



**3DEXPERIENCE®**

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# Agenda

Aspects of Digitalization in the Lab

Data Acquisition – FAIR Data

Structured vs unstructured data handling

Successful Digitalization Projects

Use Cases from the Chemical Industry

Conclusion

# Aspects of Digitalization in the Lab



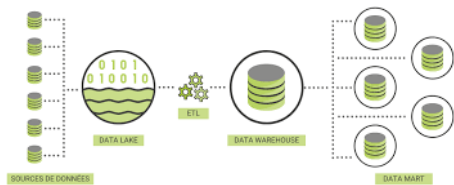
Experiments



Instruments



Data



Data Marts or Lakes



Process Optimization



Standardization



Security



Departments /Sites

# Market Trends – Goals for Digitalization



Efficiency



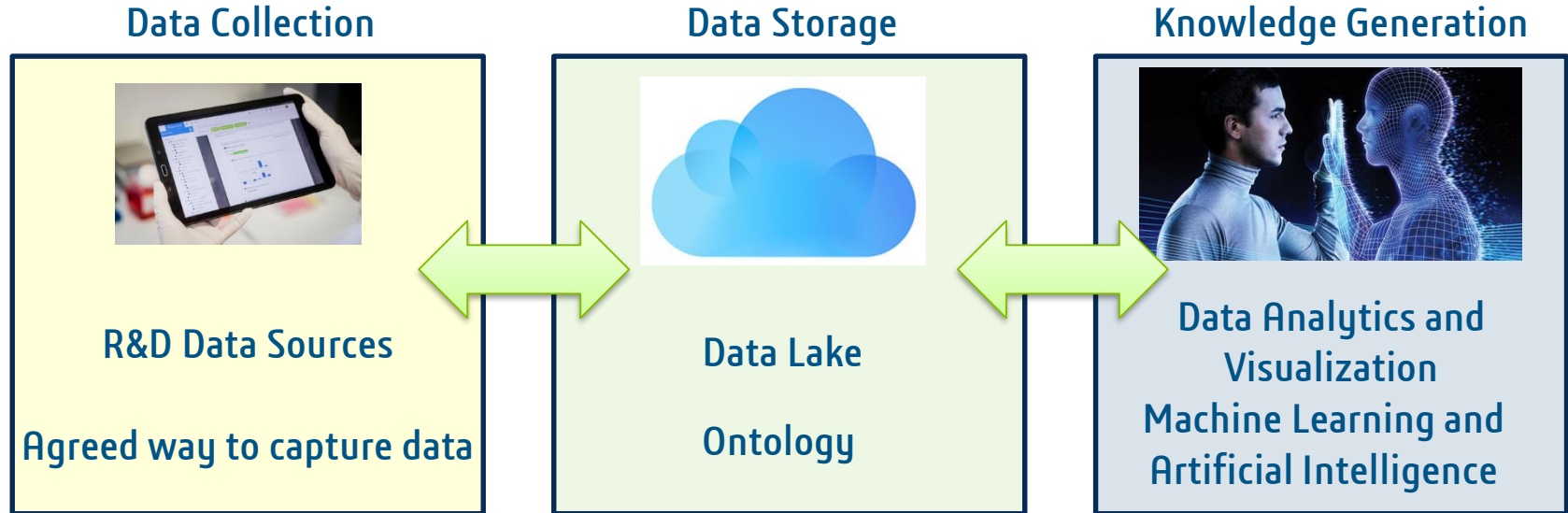
Sustainability



Innovation

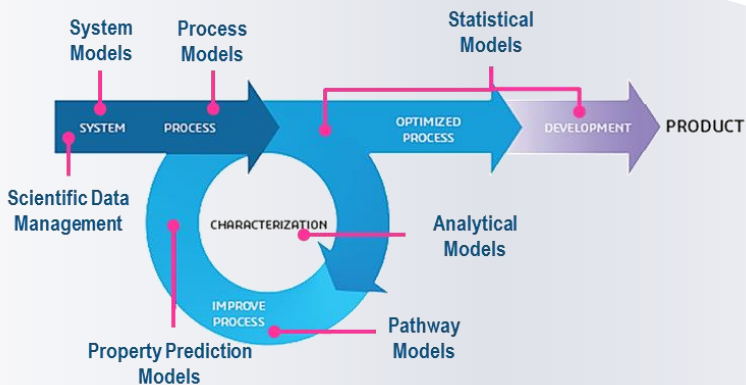
- ▶ Driven through Digitalization
  - ▷ R&D – Faster idea generation and processing
  - ▷ Through the product lifecycle – Faster time to market
  - ▷ More sustainable – Avoid unnecessary work

# R&D Digitalization – Knowledge Management



# Combining Laboratory and Simulation

## Virtual



### More Models

Explore more options faster and more cost effectively than physical equivalents



**Program Level Visibility & Coordination**

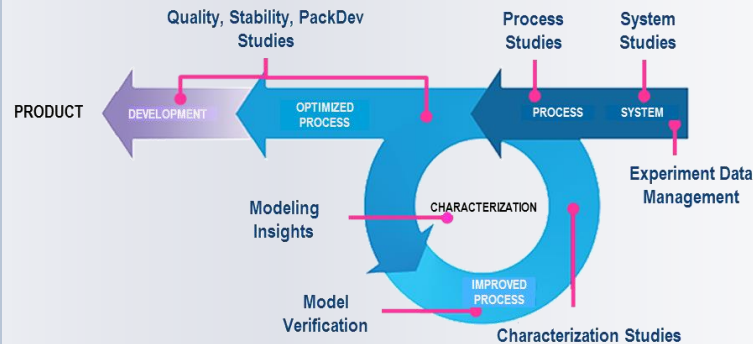
**Dark Data to Reusable Knowledge**

**Scientific Innovation Lifecycle Management**

**Scale-up & Commercialization**

**Sustainable Product Development**

## Real



### Less Testing

Avoid costly routine and duplicate studies



"I have such a hard time finding old data that it's just easier to redo the experiment..."



Poor Approach to Cross-Department Communication

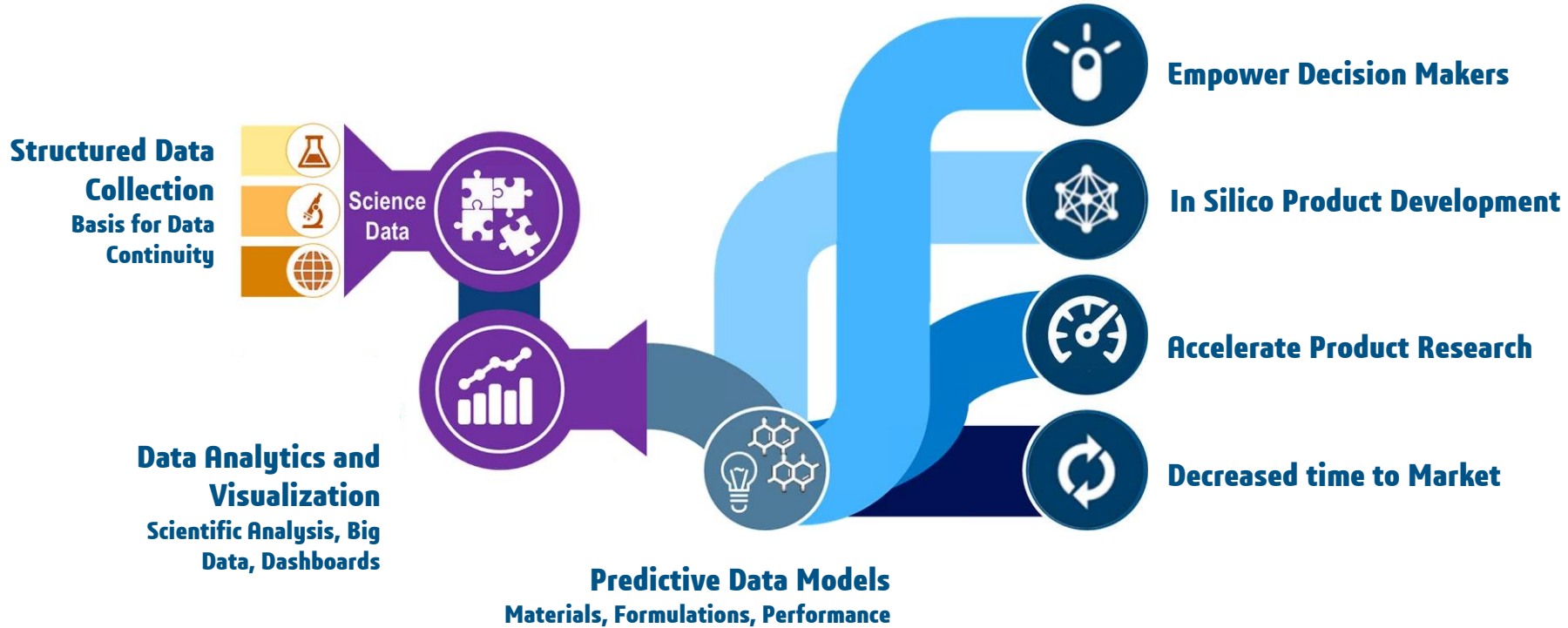


Lack of Project Coordination Infrastructure



Undocumented Siloed Scientific Intelligence

# Scientific Innovation Support – From Data to Model





# What most of our customers face today

## Lots of Data - Sometimes handwritten

- Raw Data files
- Summary data of a single experiment ends up in an Excel sheet
- Many data files are stored locally
- Or on SharePoint or File Shares
- But, is this FAIR data?

Formulation Name	Form 1	Form 2	Form 3	Form 4	Form 5
Formulation Notes	Notes 1	Add Dry A	Add more	Based on	1 Adding A
Batch Size	100g	100g	100g	20g	100g
Materials	Material IDs	Active Ingredient	Process Aid	Process Aid	Process Aid
M123	10 mass%	15 mass%	15 mass%	15 mass%	15 mass%
M456	20 mass%	20 mass%	4 mass%	20 mass%	20 mass%
M789	5 mass%	5 mass%	5 mass%	5 mass%	5 mass%
M1234	1 mass%	5 mass%	5 mass%	5 mass%	5 mass%
M5678					2 mass%

Handwritten notes on paper:

Agglutination von [redacted] (ca. 10 S.H.) mit ALP [redacted]  
 25% Überschub; so [redacted]; [redacted]  
 Anschließend Umlagerung ALP-Prozentrif-PE zum Profing, baldigst  
 200g 200g 200g 200g 200g ALP [redacted] 200g  
 120,2 g/kg  
 250g 200g  
 100g 200g  
 100g 200g

Einzelmengen

1) 88,15 g [redacted] ES 1317 [redacted] 0,94 g S.H./kg; [redacted] g/kg = 0,083 kg  
 2) 61,85 g ALP [redacted] ES 2252 [redacted] 12,102; 591,17 g/kg = 0,104 kg, 25%  
 3) 75 ul [redacted] P. 1. v. 22.11.12 = 5 ppm PE  
 [redacted] = ~ 0,5%  
 [redacted] = ~ 0,25%

29.01.13  
 → 4h; bei 54°C (kol 3) unter  
 nach 30 min Gesamtkaltransit auf  
 weiteren 10 min; Kühlung mit HeiS  
 100% Umrats  
 11  
 30.01.13  
 Probe warm über 150% Fei →  
 nicht mit durch (etwas)  
 Probe warm über 535 1/2 Fei →  
 lange → anheben klar  
 136 145 g, Jan 31/2011  
 br klein cis + trans Propenyl-PC  
 rhyd

Screenshot of a data table with handwritten annotations:

Sample	G	H	I	J	K
Sample 1	20.0	20.0	20.0	20.0	20.0
Sample 2	15.0				
Sample 3		12.0			
Sample 4			6.0		
Sample 5				6.0	
Sample 6					45.0
Sample 7	45.0	45.0	45.0	45.0	45.0
Sample 8	120.0	120.0	120.0	120.0	120.0
Sample 9	200	200	200	200	200
Sample 10	5.0%	5.0%	5.0%	5.0%	5.0%
Sample 11	10.0%	10.0%	10.0%	10.0%	10.0%

# Data Acquisition – FAIR Data

There are 4 guiding principles of FAIR Data:

**F**

**Findable**

Data and supplementary materials have sufficiently rich metadata and a unique and persistent identifier.

**A**

**Accessible**

Metadata and data are understandable to humans and machines. Data is deposited in a trusted repository.

**I**

**Interoperable**

Metadata use a formal, accessible, shared, and broadly applicable language for knowledge representation.

**R**








**Reusable**

Data and collections have clear usage licenses and provide accurate information on provenance.

# How do we get to FAIR data?

- ▶ Good STANDARDIZED, high quality Data
  - ▷ Clean comparable data is the basis
- ▶ Same Ontology
  - ▷ Same name for the same things – e.g. Density vs Spec. Gravity
- ▶ Same Units of Measure
  - ▷ Same units e.g. Gramm, G, g
- ▶ Normalization
  - ▷ Common base for all measured properties e.g. degree Fahrenheit vs Celsius
- ▶ Storage in a structured way
  - ▷ Data must be easily retrievable - from all scientists - on all experiments
  - ▷ Data must be FAIR

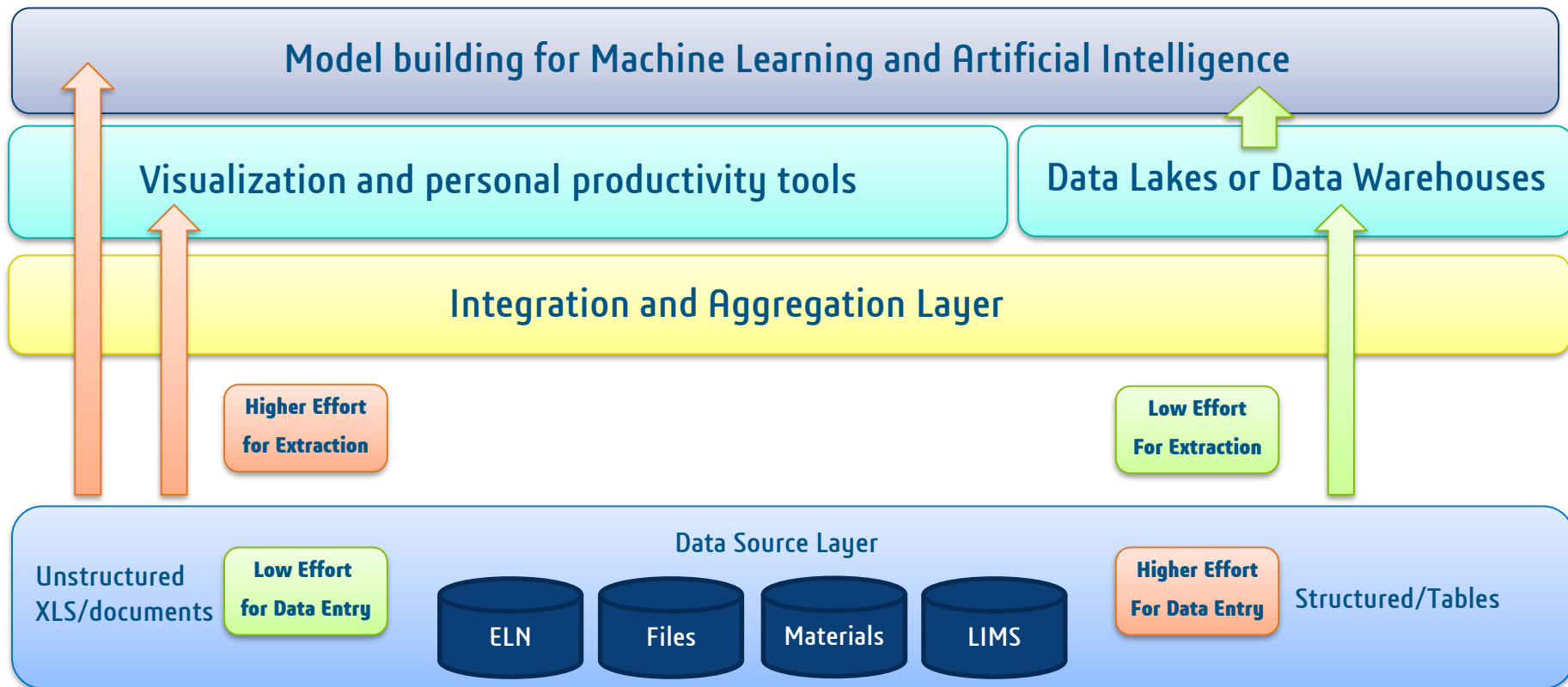


Physical quantity measured	Base unit	SI abbreviation
	mole	mol
	meter	m
	kilogram	kg
	second	s
	kelvin	K
	ampere	A
	candela	cd





# Data Organization



# What do successful Digitalization projects look like?

- ▶ Looking at optimizing the experimentation processes ✓
- ▶ Easy collection of standardized data ✓
- ▶ Fully integrated – Workflows, Instruments, Resources ✓
- ▶ Driven by the whole organization ✓
- ▶ Providing data access security ✓
- ▶ Scientific support for Scientists ✓
  
- ▶ **Start with the end in mind** ✓
- ▶ Expertise is more important than Software ✓

# BIOVIA Lab Management Solution

## Lab Planning/Management

- Request Work
- Schedule, Review
- Confirm Requests

## Sciences

- Chemistry
- Formulations
- Analytical
- Application Testing

## Resources

- Samples
- Materials
- Personnel
- Equipment
- Chemical Registration
- Biological Registration

**Unified  
Integrated  
Standardized**

## Lab Execution

- Prepare Tests
- Perform Tests
- Assay Management

## Recipes/Methods

- Develop procedures
- Adapt procedures
- Manage procedures

## Reporting/Analysis

- Compile, Interpret Results
- Generate Reports



# Global advanced materials industry leader Evonik – SmartLab



**EVONIK**  
INDUSTRIES



## Challenge: Managing scientific research processes for global R&D

Goal	Value	Benefits
<ul style="list-style-type: none"> <li>• Central ELN needed to enable collaboration</li> <li>• Full integration of all research departments</li> <li>• Handling of all data in the lab in a B2B setting</li> <li>• Protect Evonik IP</li> </ul>	<ul style="list-style-type: none"> <li>• Support 3000 scientists in divers disciplines</li> <li>• Central repository for all R&amp;D data</li> <li>• Scientific data protected for NDA critical projects</li> </ul>	<ul style="list-style-type: none"> <li>• Reduced unproductive times for lab scientists</li> <li>• Faster product innovation</li> <li>• Secure, controlled access to information from all global labs</li> <li>• Increased IP protection for business partners</li> </ul>



# Huntsman – Increase R&D effectiveness



Challenge: Scientists collecting information on paper and files

Goal	Value planned	Benefits
<ul style="list-style-type: none"><li>• Global ELN solution needed to enable collaboration</li><li>• Support the work process of the formulators</li><li>• Collect all data in the lab in one central place</li><li>• Create a digital backbone for the laboratory</li></ul>	<ul style="list-style-type: none"><li>• Increase efficiency for 750 scientists and technicians</li><li>• Reduce data loss &amp; increase data reuse</li><li>• Improve completeness of data and facilitate collaboration</li><li>• Use of data for model building AI/ML</li></ul>	<ul style="list-style-type: none"><li>• Model based guidance for experimentation</li><li>• Reduce unproductive times for lab scientists</li><li>• Fast and easy access to all information generated across all labs</li><li>• Single source of truth</li></ul>

# Conclusions

- ▶ It is hard work to agree on standards within a scientific organization
- ▶ Digitalization is rather a business transformation than just implementing software
- ▶ Materials Science companies need to define a data analysis strategy and related technology strategy
- ▶ This strategy influences the way experiment data needs to be stored
- ▶ Dassault Systèmes provides solutions for Lab Digitalization and Product Lifecycle Management

