Coatings Trends & Technologies SUMMIT

Design and implementation of a digitalization strategy for coatings industrial research and development

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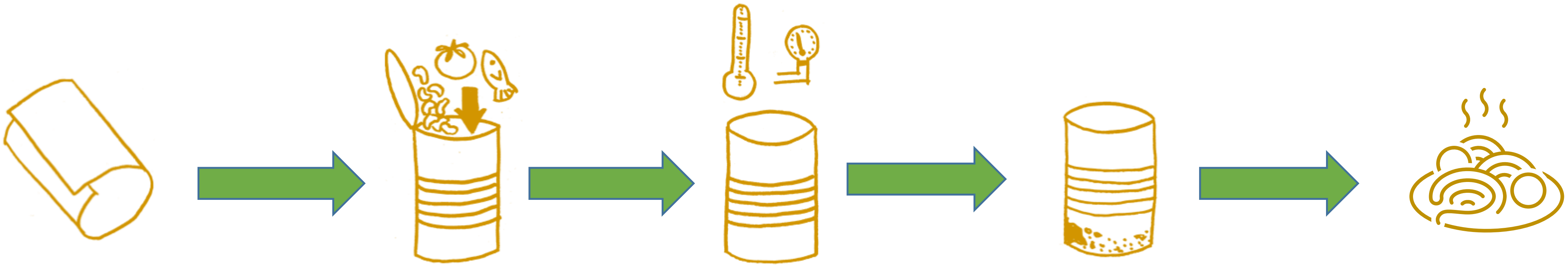
Metal packaging coatings undergo a lot of stress



Large deformation on coated metal sheets

Direct contact with aggressive food

Food sterilization at 120 – 130 °C

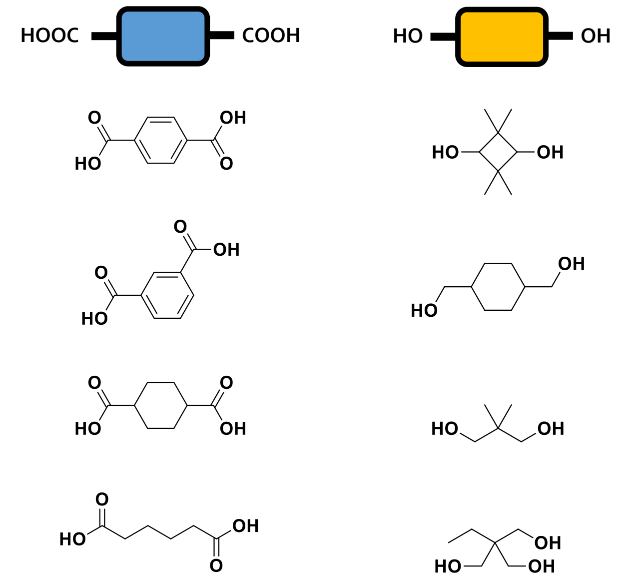
2 – 3 years shelf life

Fresh tasting food

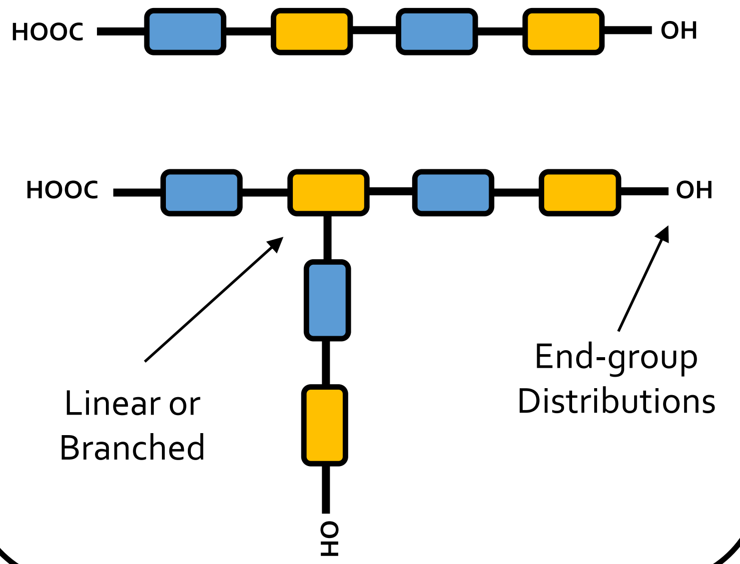
Source:
Food Packaging Forum: https://www.foodpackagingforum.org/food-packaging-health/can-coatings

Complex design spaces

Compositional



Structural



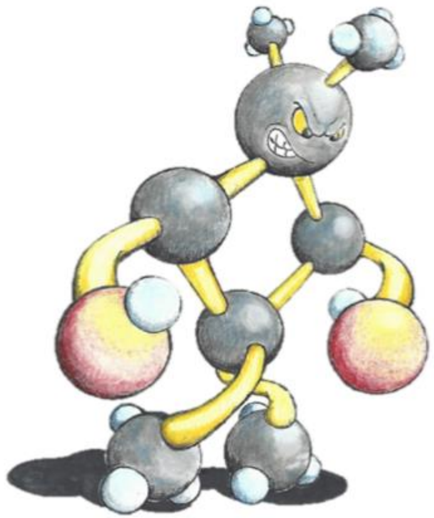
Balance of Properties

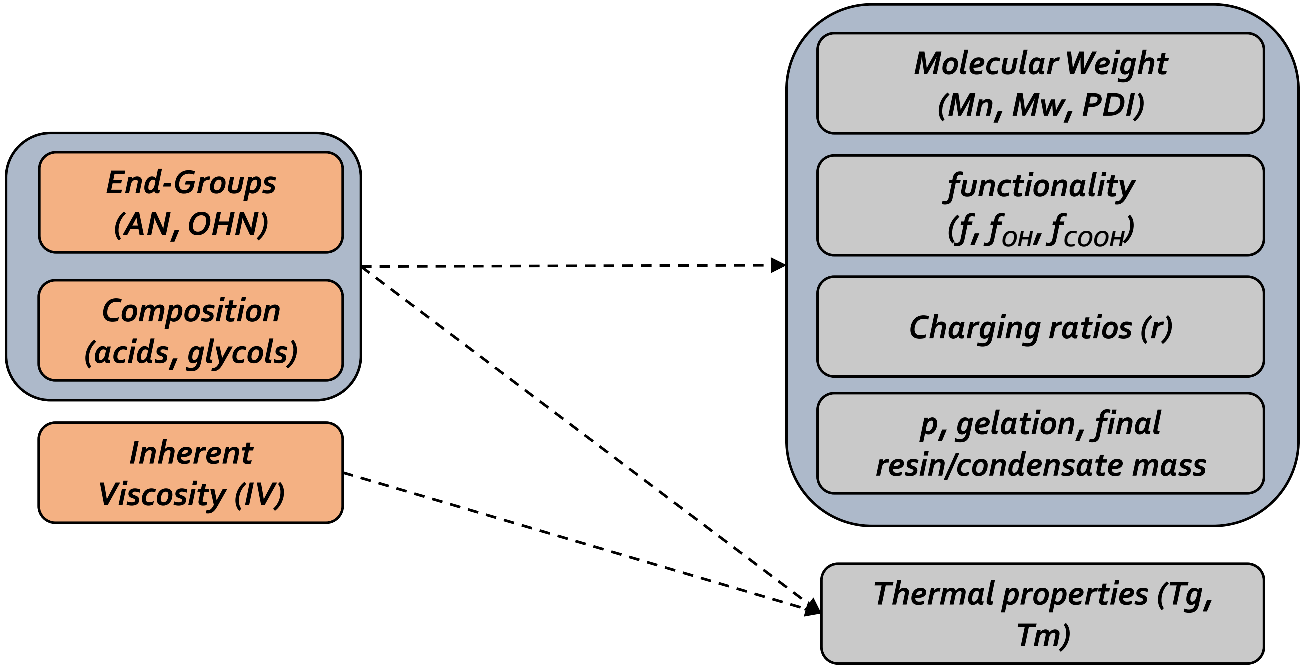
- Thermal (Tg, Tm)
- Viscosity/Molecular Weight
- Reactivity
- Solubility

**polyesters act as the main binder; however, formulations also include added crosslinkers, solvents, catalysts, and various other additives*

Inputs
Outputs

Modeling via first principles

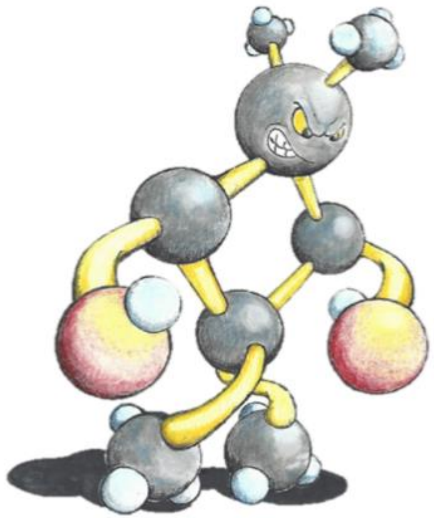


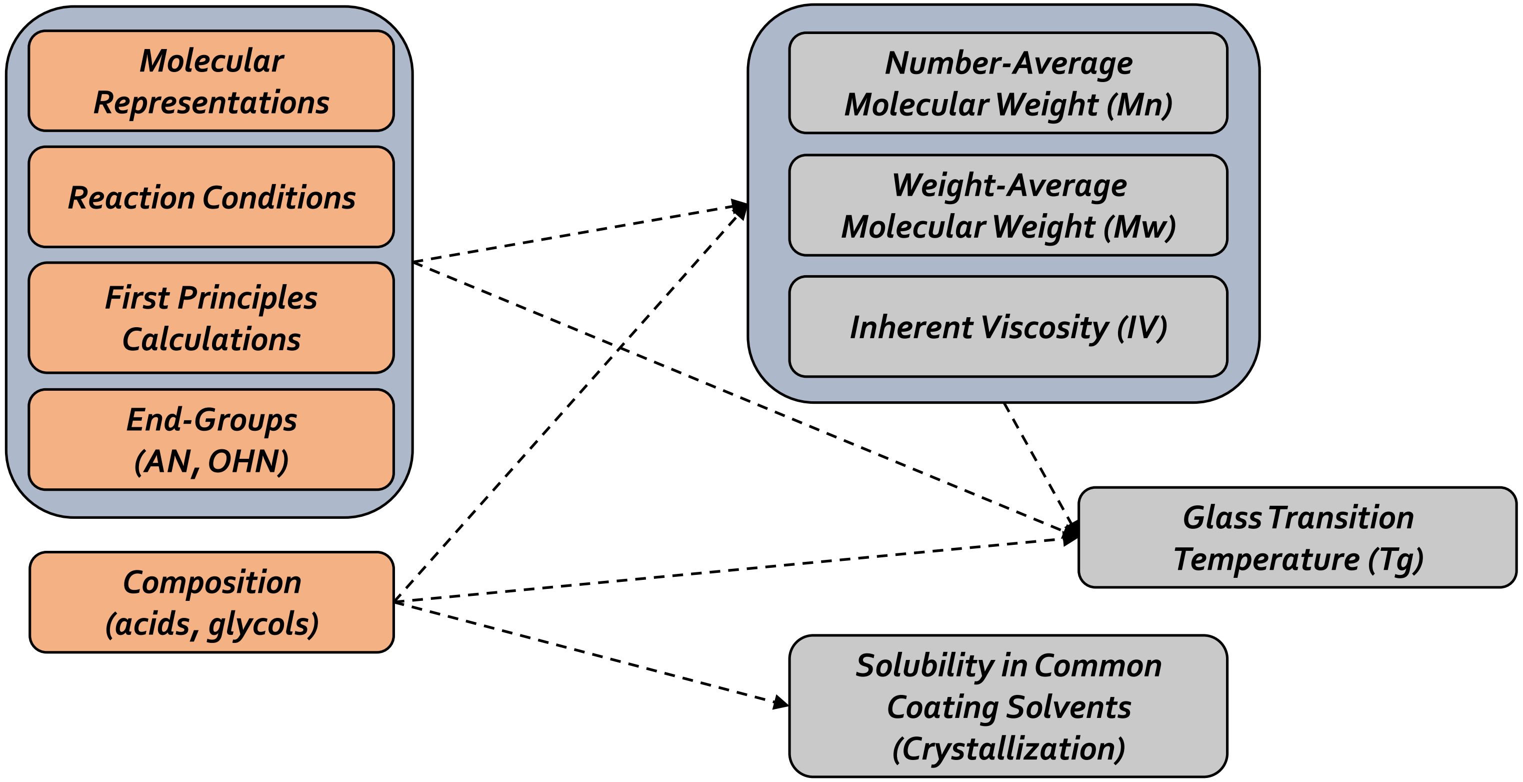


Flory, P., Chem. Rev. 1946, 39, 1, 137-197
Stockmayer, W., J. Polym. Sci. 1952, 9, 1, 69-71

Modeling via machine learning

Inputs
Outputs





**all models are random forest (classifier for crystallization and regression for everything else)*
**rows with missing outputs are filtered out before prediction*

Stacking models together

Base Resin Models

Inputs
- Composition
- End-groups
- Etc.

Flory I →

Resin Properties
- Tg
- MW
- IV
- Etc.

Flory II →

Coating Properties
- MEK DR
- Wedge Bend
- Retort
- Etc.

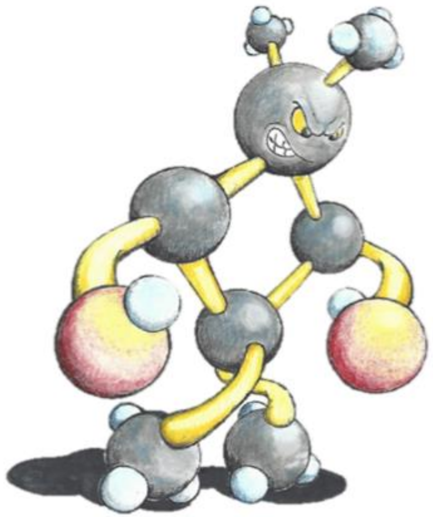
Flory X ↓

Base Formulation Models

Inputs
- Resins
- Crosslinkers
- Additives
- Etc.

Flory III →

Coating Properties
- MEK DR
- Wedge Bend
- Retort
- Etc.



Queen, O., McCarver, G.A., Thatigotla, S., Abolins, B.P., Brown, C.L., Maroulas, V., Vogiatzis, K.D. Polymer graph neural networks for multitask property learning. npj Comput. Mater, 9, 90 (2023).
McCoy, S., Ojedeji, D., Abolins, B., Brown, C.L., Doxastakis, M., Sgouralis, I. Quantitative Structure-Property Relations for Polyester Materials via Statistical Learning. Macromol. Theory Simul. 2024, 33, 2400008.

But the data…

- Scattered among dozens of scientists, lab notebooks, technical reports, spreadsheets, etc.

- Poorly organized and lacks any standardization

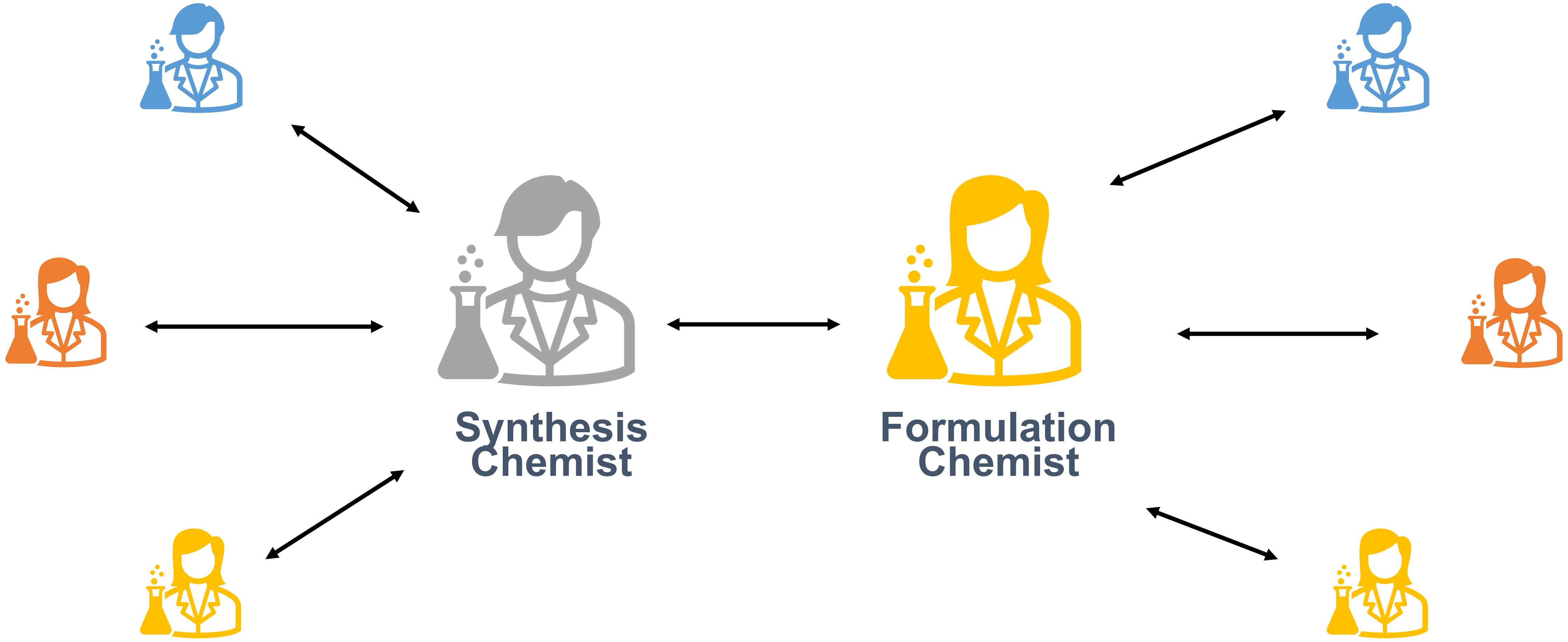
- Errors and typos

- **NOT:**
    - **F**indable
    - **A**ccessible
    - **I**nteroperable
    - **R**euseable

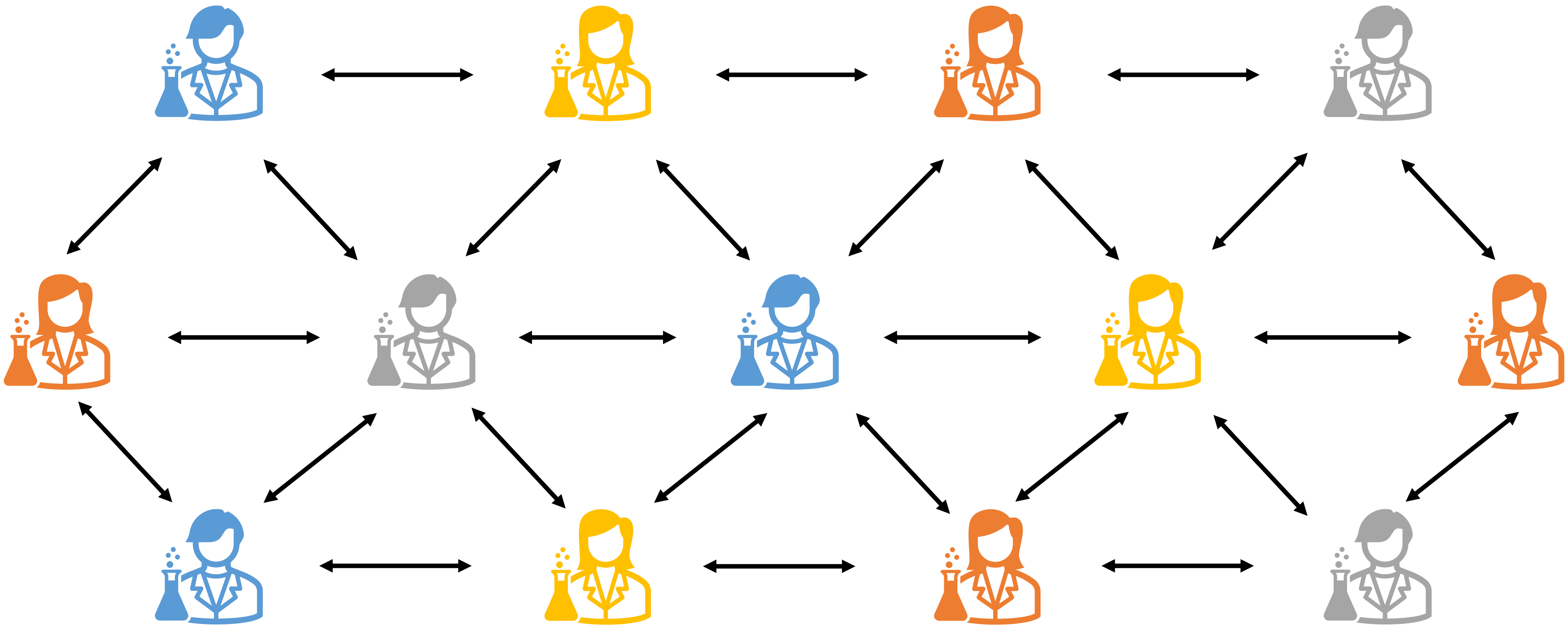
- Getting data right is the next step

Wilkinson, M., Dumontier, M., Aalbersberg, I. *et al. Sci Data* 2016, 3, 160018.

R&D at a large chemical company

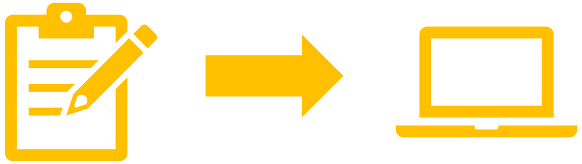


R&D at a large chemical company



A bit of history

- Paper to e-notebooks



- 2013: US went from first to invent to first to file

- 2020: Pandemic induced digital acceleration

We've adopted many digital tools

UCaaS (Microsoft Teams, etc.)

Notebooks

Laboratory Information Management System

Technical Reports

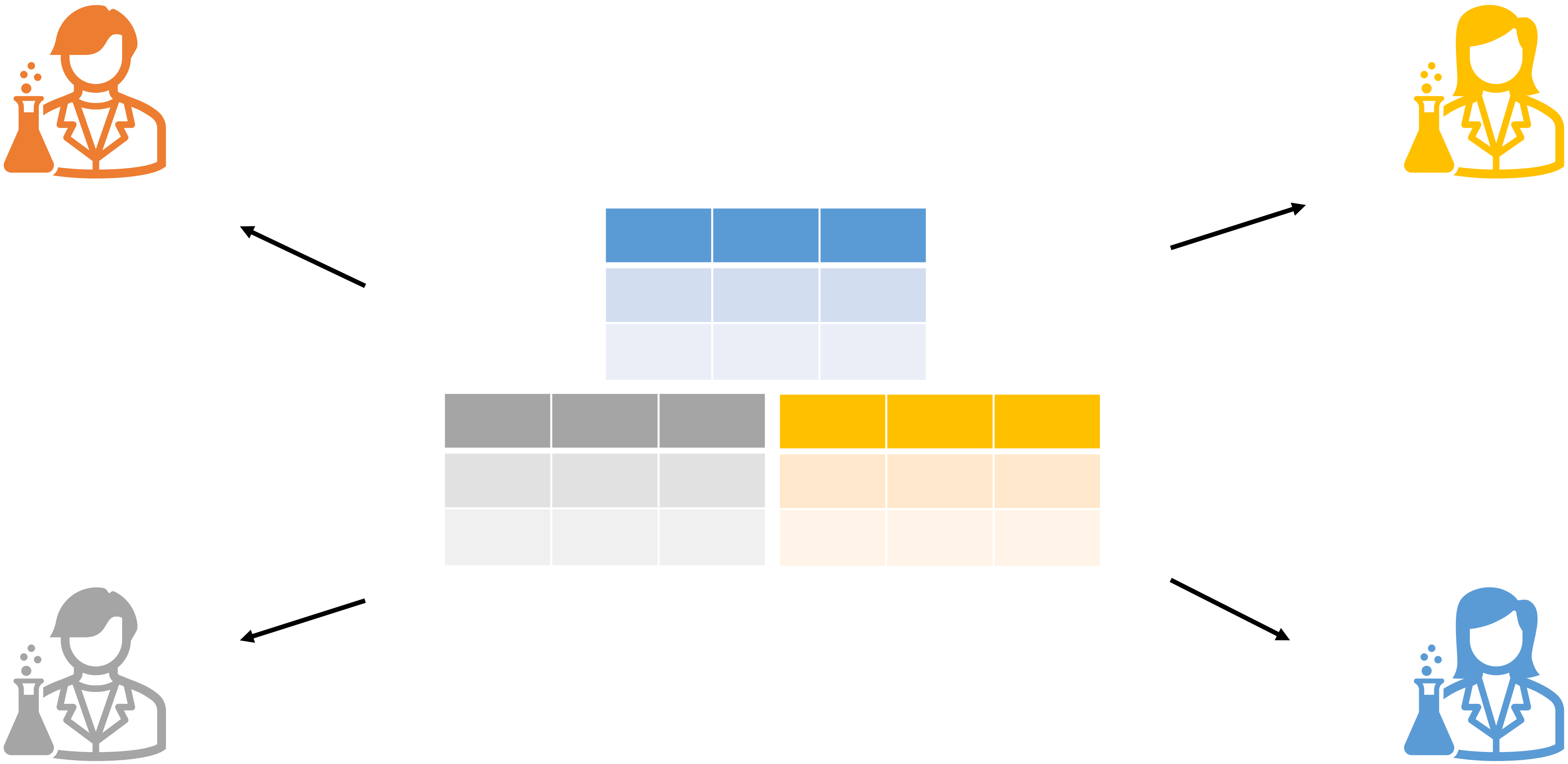
Chemical Inventory Management Systems

Project Management Systems

What do we want to do?

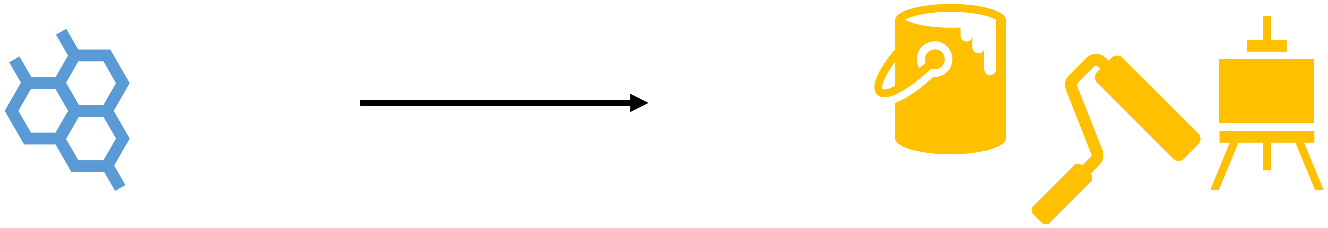
- Eliminate redundancy and clutter
- A system that makes it easy to create, organize, store, and retrieve data
- Reduce errors in the data
- Build a culture that prioritizes and rewards data organization

Master Data Tables



Rethinking how data is collected: F.A.I.R.

From:



Resin

Paint/Panel

- Exp. data siloed in individual notebooks/files
- Shared excel files used to gather larger trends, but inefficient, redundant, and error prone
- Naming entities not consistent b/t teams or experimental sets

Rethinking how data is collected: F.A.I.R.

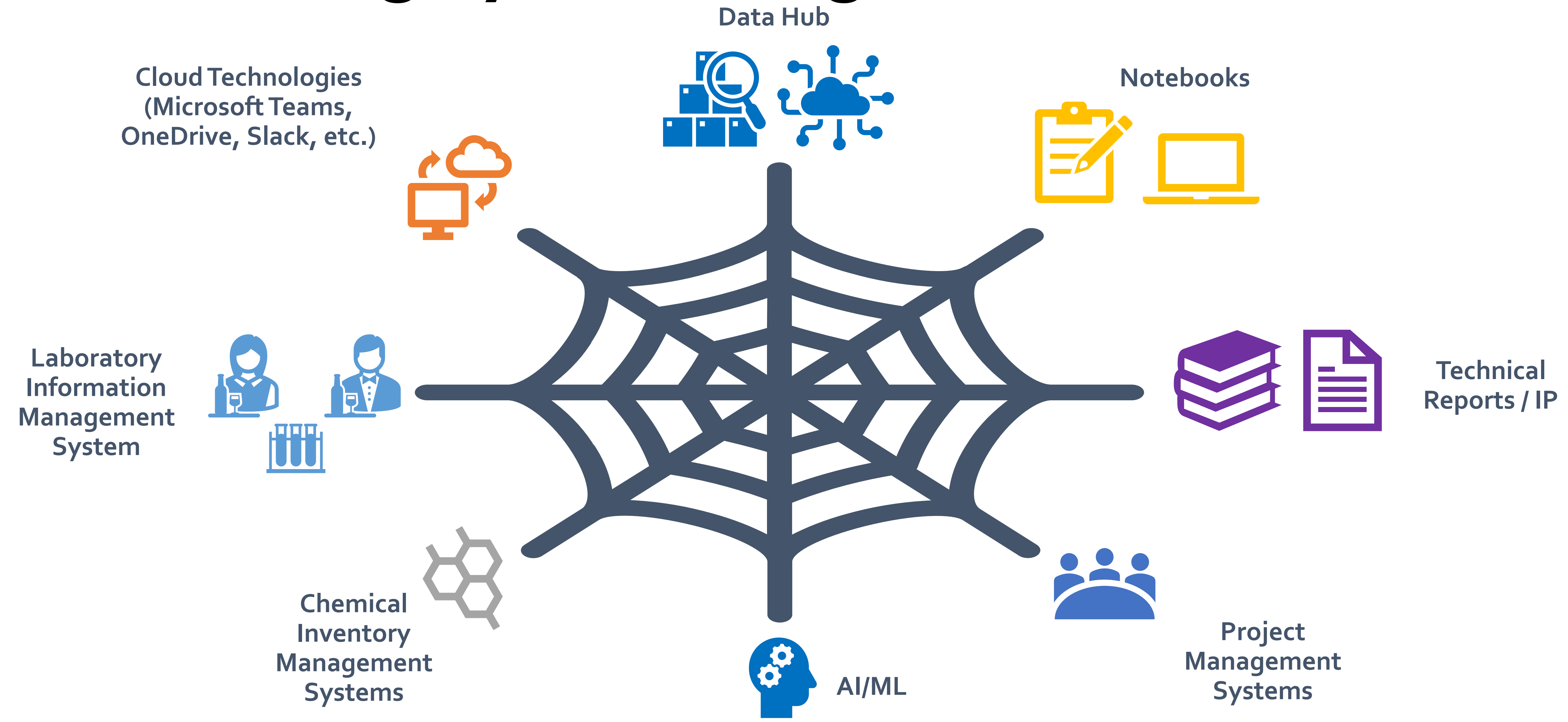
To:

Resin Paint Panel

- Establish formal relationships between data
- Each discreet material gets a unique identification number

UniqueID	Descriptor1	Descriptor2	Descriptor3	Property1
1				
2				
3				

Connecting systems together



Barriers and outlook

- Change is hard
- Everyone is busy on today’s emergency
- Many ways to organize
- Our business units are similar, yet different
- Still looking for the right combination of tools
- It’s along journey, stay motivated

Questions?

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