



materials design

WEBINAR

Advancing Automotive Innovation with Materials Modeling

Jonathan E. Mueller, Ph.D.
Volkswagen AG



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Audio

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Talking: Katherine Hollingsworth

Questions

Q: Can you calculate the gelation point of a polymer?

A: Yes we can! David will address this on an upcoming slide soon.

What forcefields are supported by MedeA?

Send

Webinar Speakers



Dr. Volker Eyert

Materials Design



Dr. Jonathan Mueller

Volkswagen AG



Katherine Hollingsworth

Materials Design



materials design

WEBINAR

Advancing Automotive Innovation with Materials Modeling

Jonathan E. Mueller, Ph.D.
Volkswagen AG

Advancing automotive innovation with materials modeling

Jonathan E. Mueller

Materials Design Webinar, April 29, 2021

Advancing automotive innovation with materials modeling

Objectives

- The main objective of this webinar is to identify the **requirements** of **industrial end users** for **materials modeling software** in order to suggest guidelines for future software development and best practices for industrial use.

Outline

1. What kind of **industrial end user** is the **Volkswagen Group**?
2. What do we use **materials modeling software** for?
3. What **requirements** do we have for materials modelling software?



Group statistics

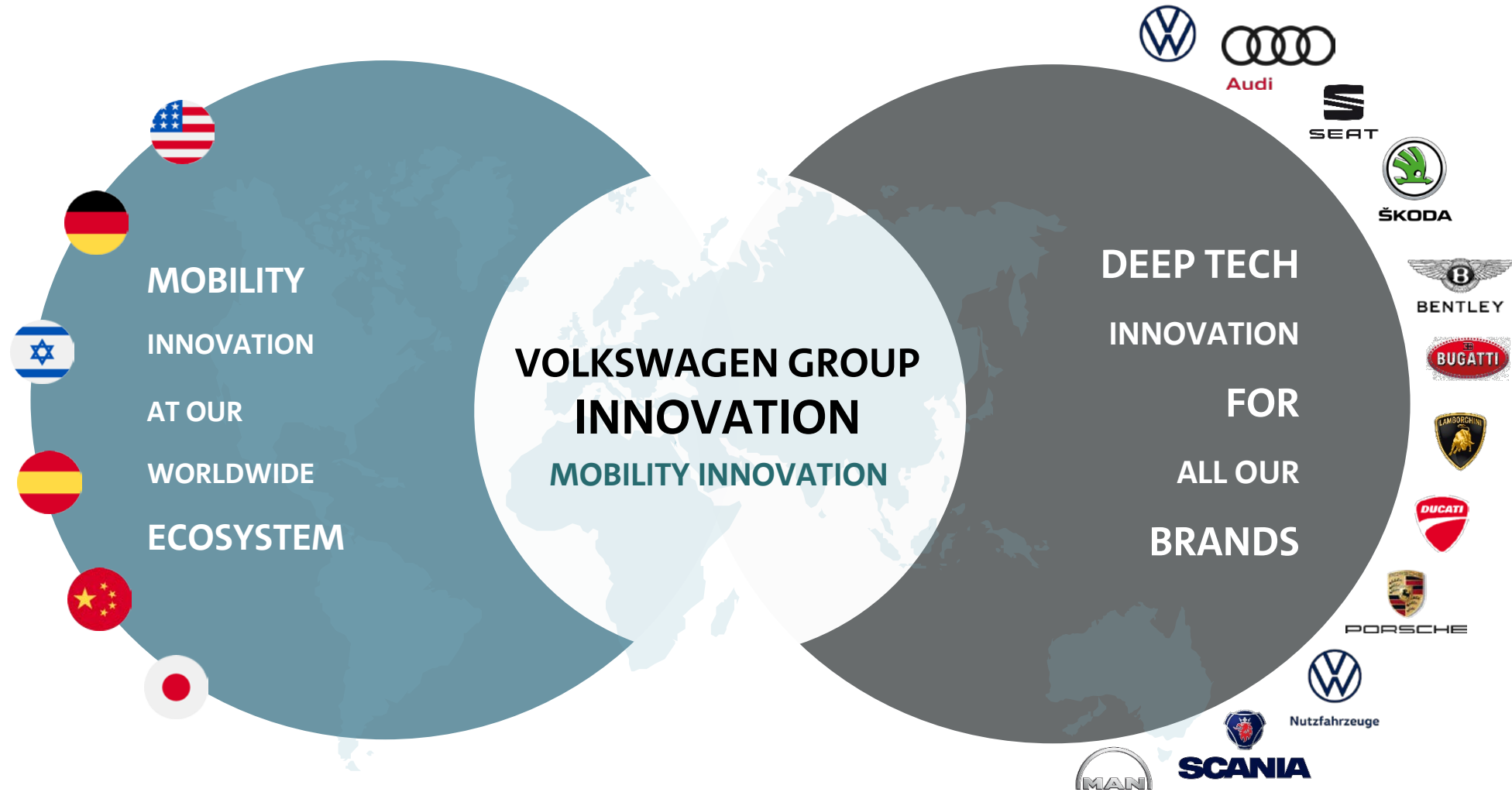
- 670,000 employees
- 125 production sites
- 43,000 vehicles per day
- 12 brands
- 365 models

Volkswagen Group

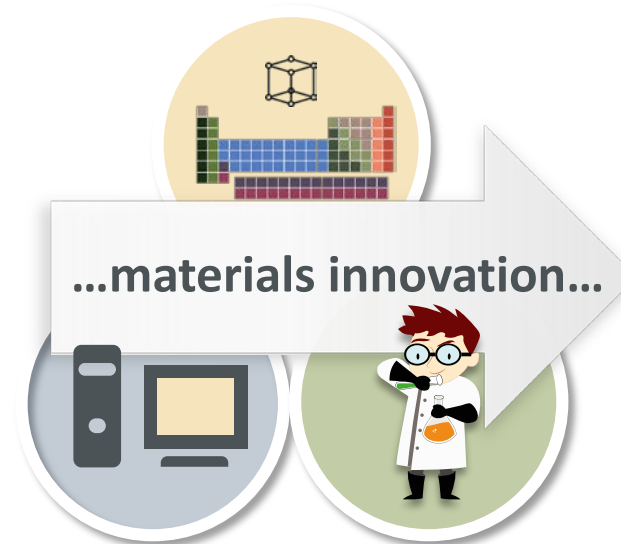


International Innovation Ecosystem

Regional Mobility & Innovation Ecosystems for and with our brands



Technological progress requires...

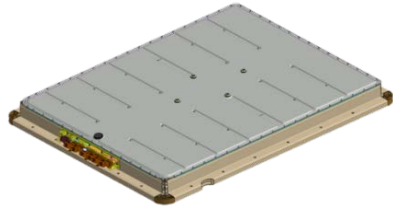


...materials innovation...

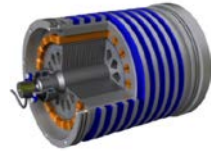


...and is accelerated by materials modeling.

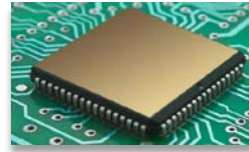
Innovative materials needed for...



battery



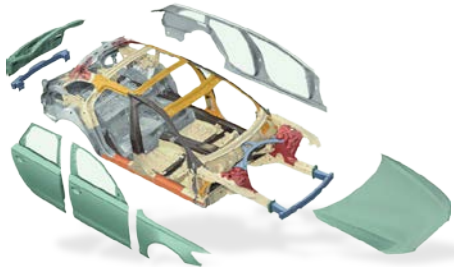
electric motor



electronics



fuel cell system



frame & body



interior

...and many other automotive applications!

Advancing automotive innovation with materials modeling

Objectives

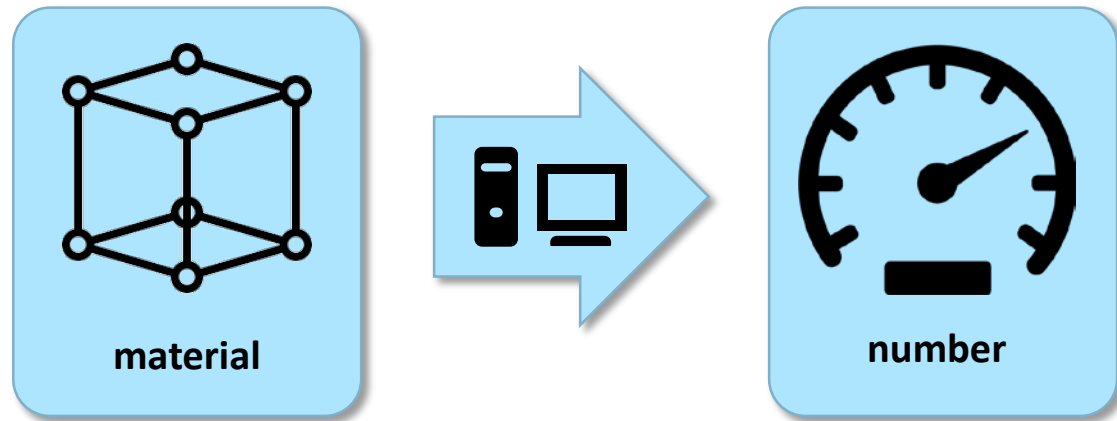
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Outline

1. What kind of **industrial end user** is the **Volkswagen Group**?
 - **Large, international** organization
 - Major **automobile manufacturer**
 - Products utilize **numerous, diverse materials**
2. What do we use **materials modeling software** for?
3. What **requirements** do we have for materials modelling software?

Materials engineering: numerically correct

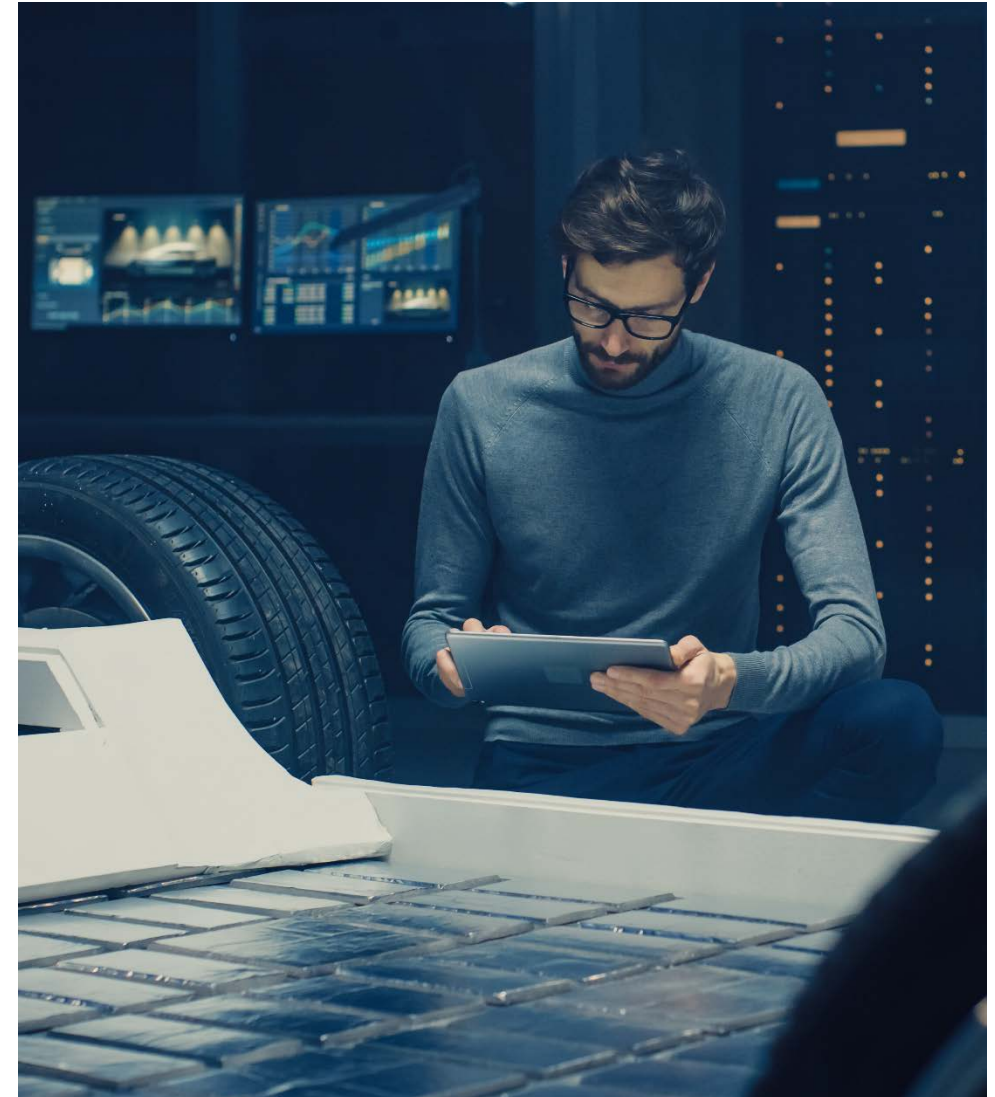
Approach: replace *quantitative* experiments with materials modeling



Requires: *numerically correct* results

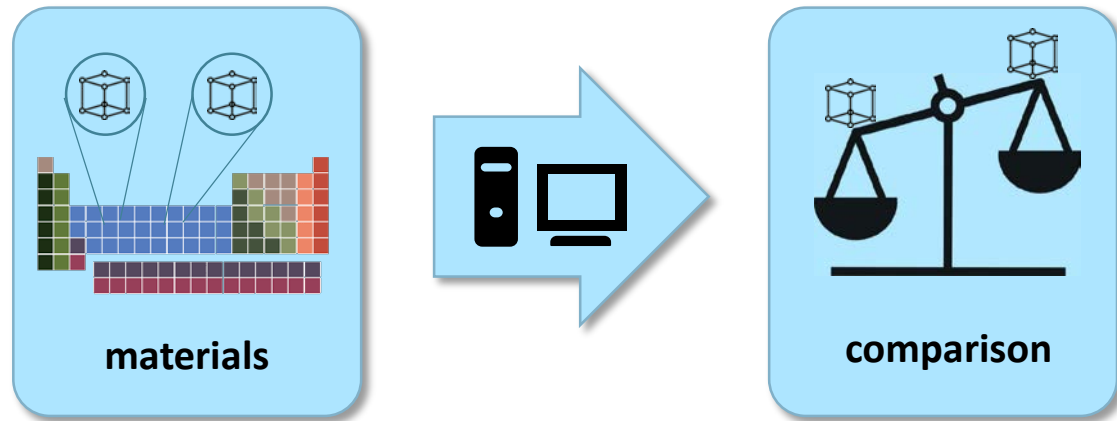
Examples:

- Generate parameters for larger scale models (*e.g.* battery aging)
- Optimize a material or manufacturing process (*e.g.* pore structure)



Materials exploration: categorically correct

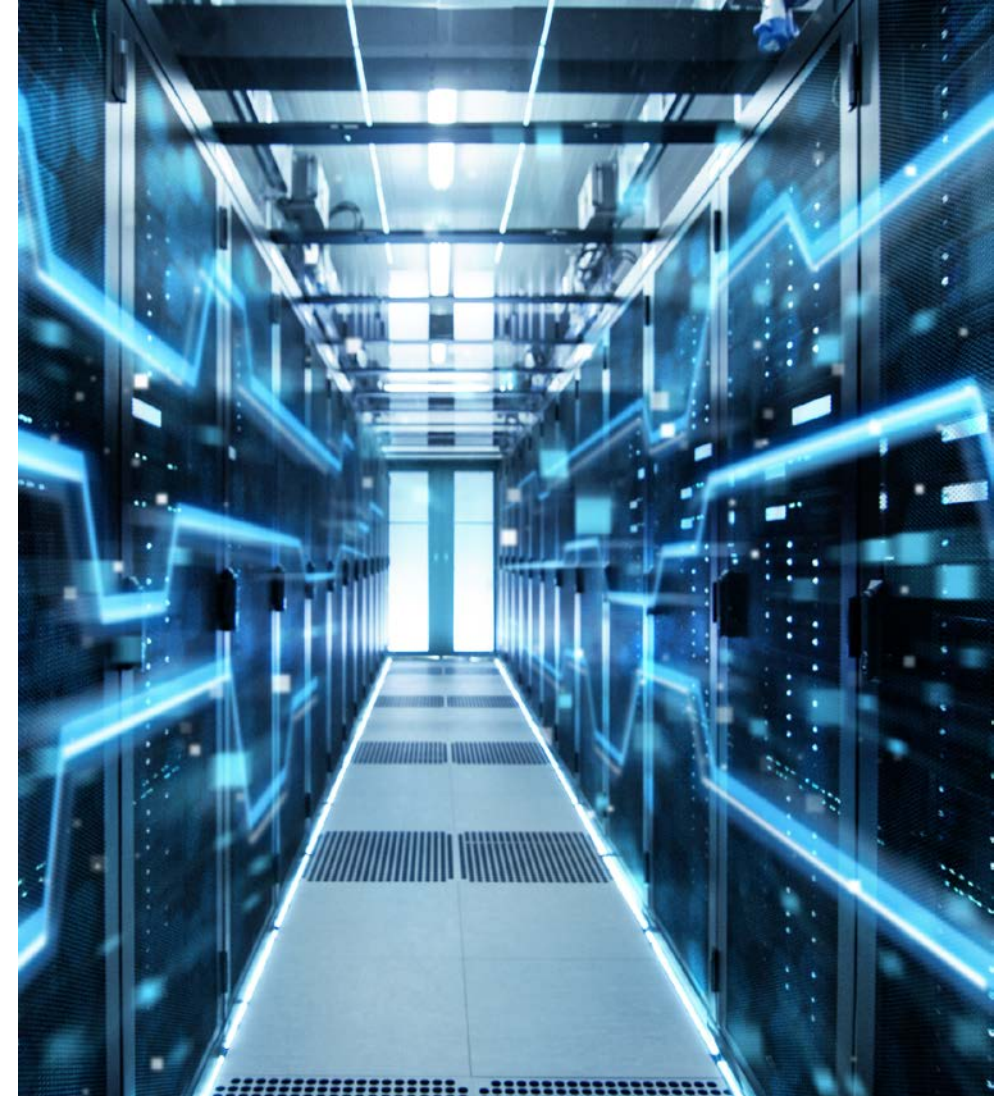
Approach: replace *screening* experiments of candidate materials



Requires: *categorically correct* results

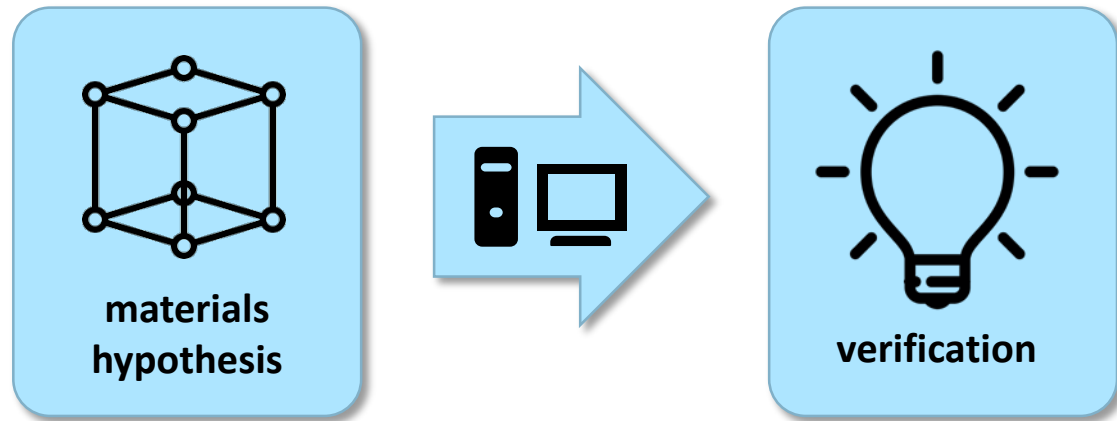
Examples:

- Search for materials exhibiting specific properties (*e.g.* hydrogen storage)
- Probe the relationship between a material's structure and its properties or performance (*e.g.* microstructure of battery cathode materials)



Materials evaluation: conceptually correct

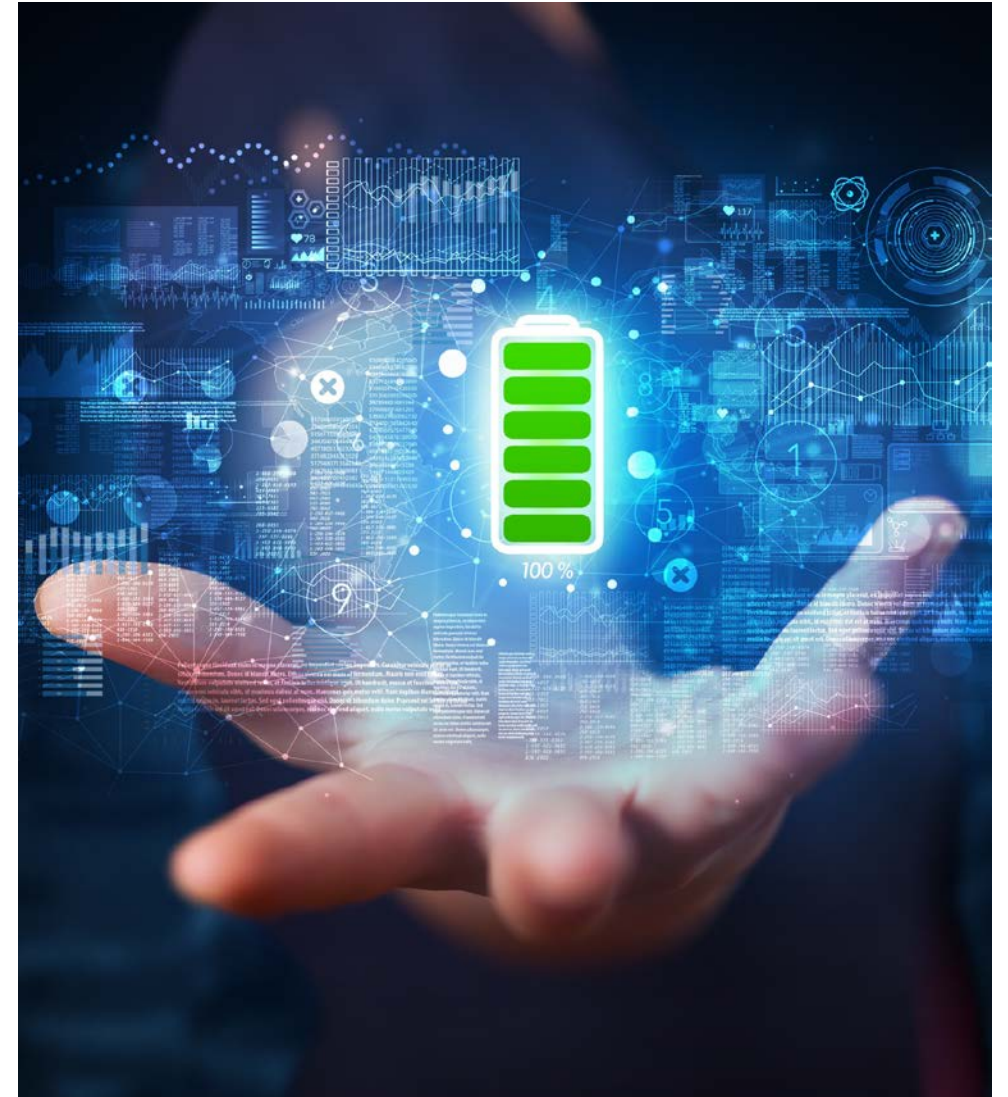
Approach: replace experiments *verifying* a materials hypothesis.



Requires: *conceptually* correct results

Examples:

- Establish plausibility of a technological approach (*e.g.* doesn't violate the laws of thermodynamics)
- Elucidate underlying physical principles (*e.g.* catalytic mechanism)



Advancing automotive innovation with materials modeling

Objectives

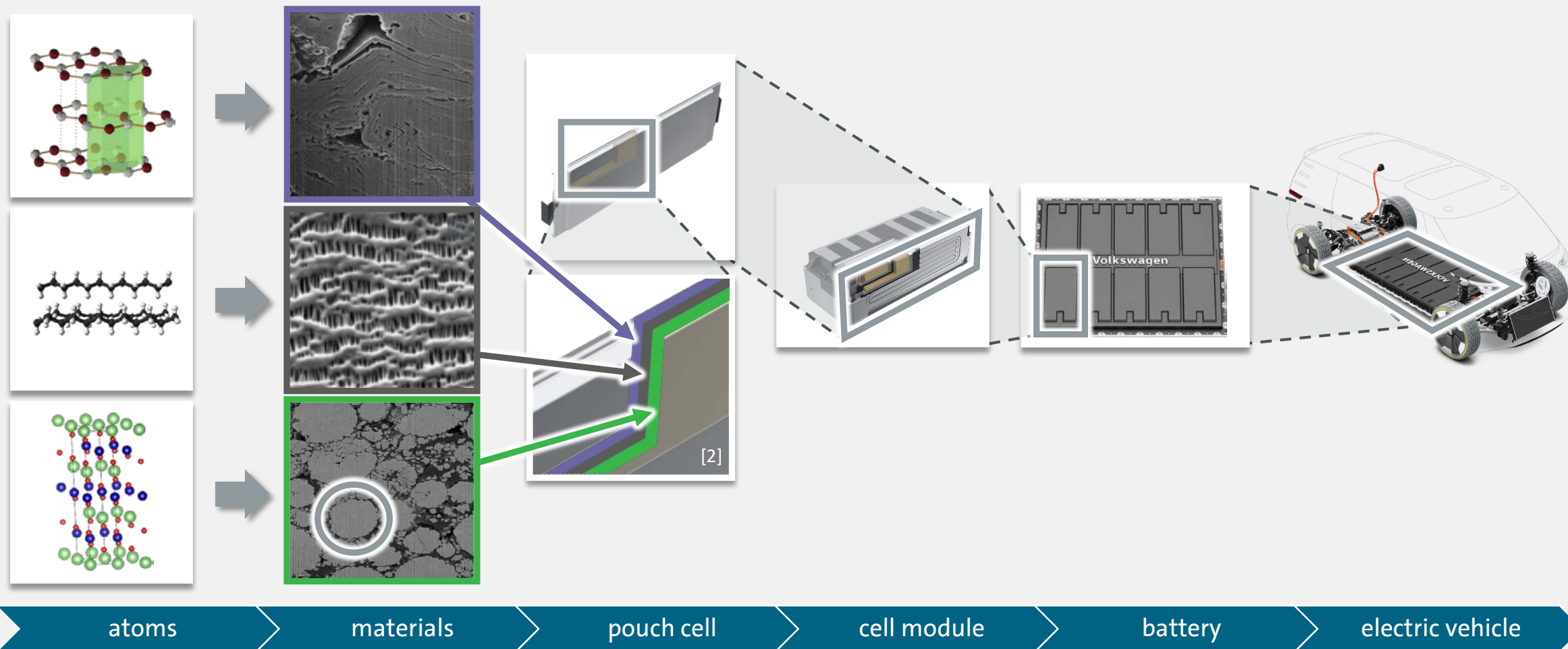
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2. What do we use **materials modeling software** for?
 - Engineering – **numerically** correct results
 - Exploration – **categorically** correct results
 - Evaluation – **conceptually** correct results
3. What **requirements** do we have for materials modelling software?

Multiscale framework

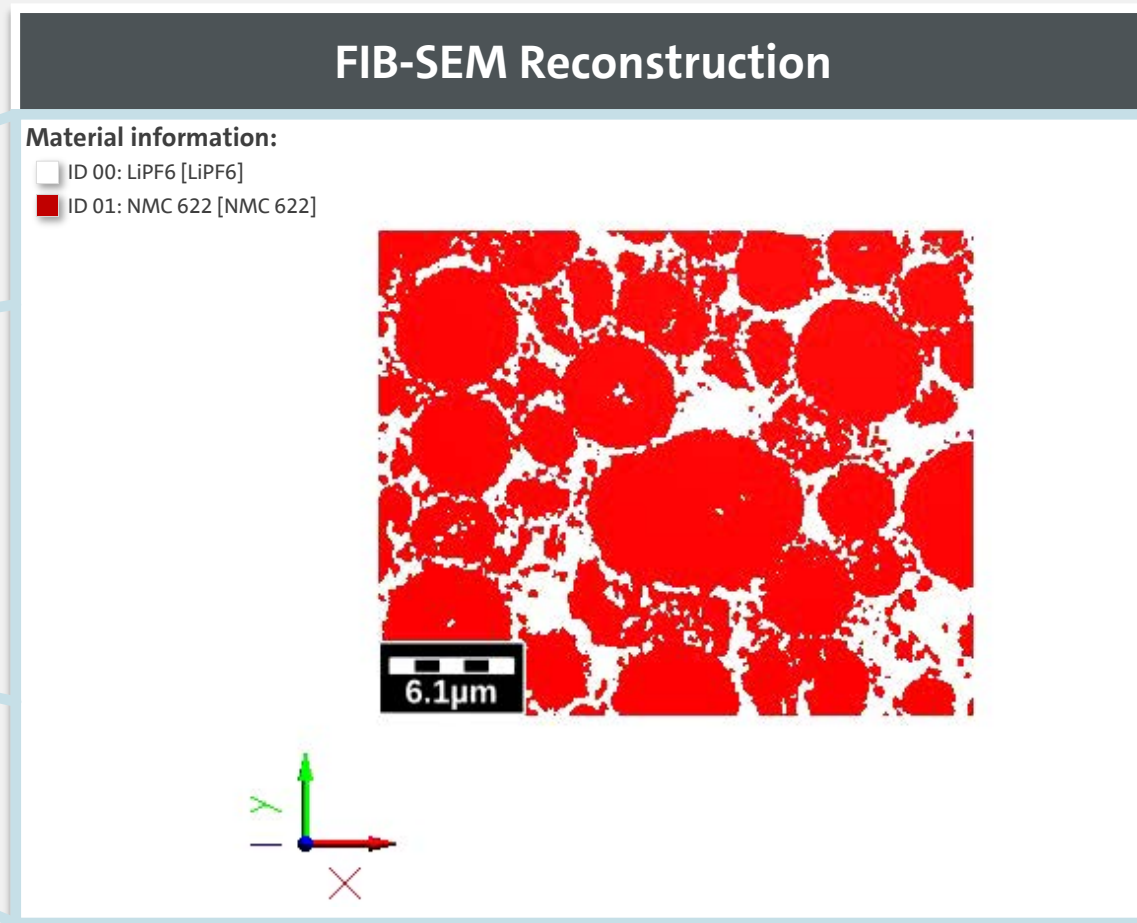
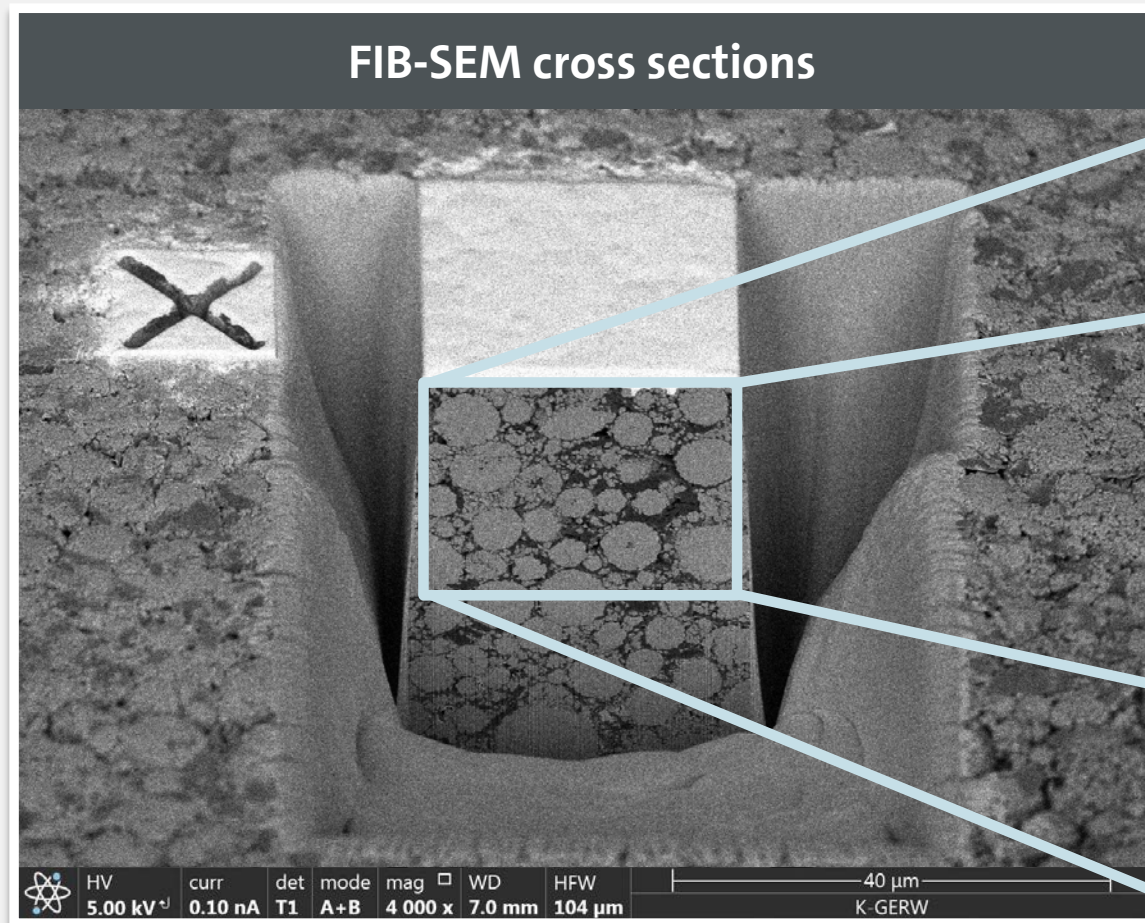
Because technology simultaneously utilizes phenomena at a range of scales...



... materials modeling software should be compatible with a multiscale framework.

Technological context

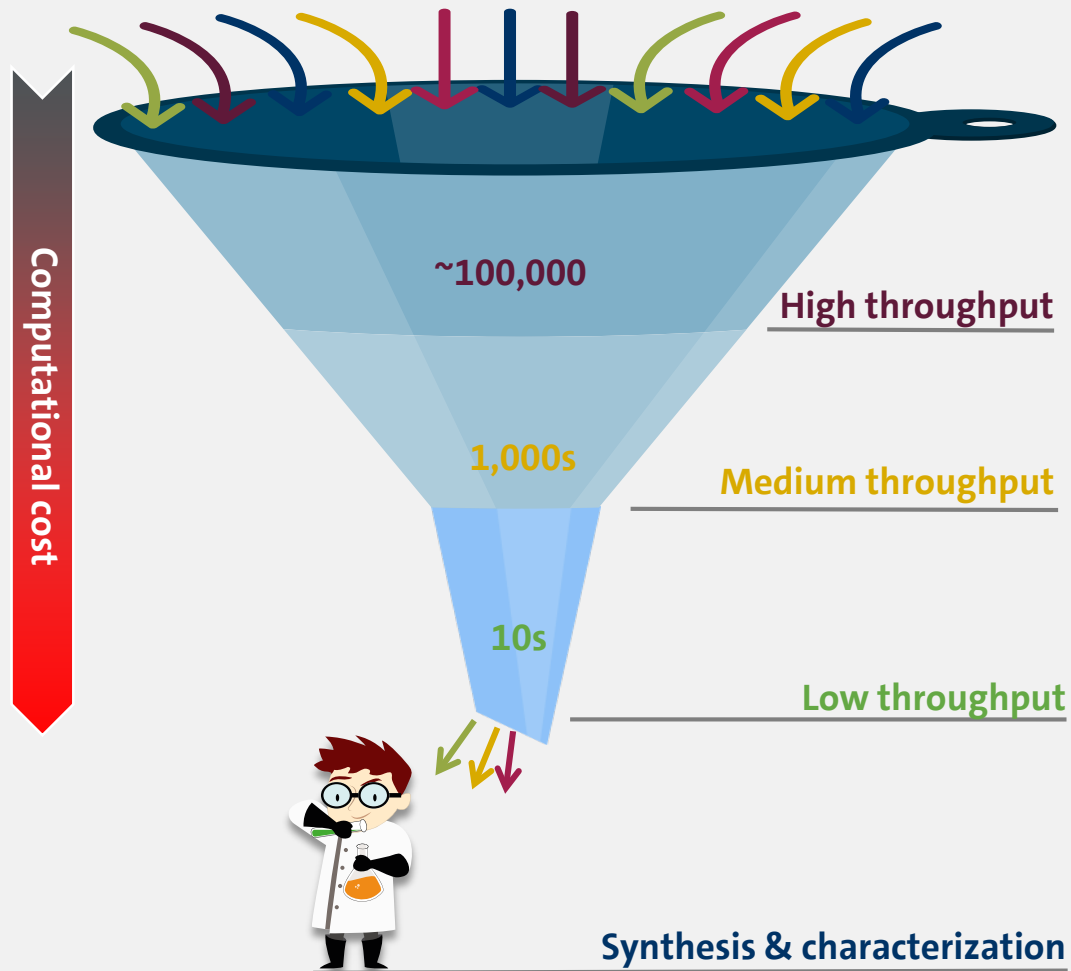
In order to apply materials in automotive technologies...



... materials modeling software should be compatible with real-world applications.

Digital environment

To utilize the many available materials databases and simulation & analysis tools...



By searching **databases** of results from previously performed simulations and experiments, more material candidates can be considered than one could feasibly test explicitly.



By performing computationally **inexpensive calculations**, a large pool of materials candidates can be efficiently pared down by ranking candidates based on one or more properties.



By performing computationally **intensive simulations**, a pool of select materials can be carefully investigated to identify the most promising candidates for synthesis.



By only **synthesizing** materials after they have been rigorously investigated computationally, the chance of finding suitable materials increases significantly.

...materials modeling software should be compatible with these tools.

Organizational boundary conditions

The best materials modeling software is useless for industry unless...



Document the use of third party software meticulously.



Build in safeguards as needed to guarantee data protection.



Design software to be compatible with network security measures.



Provide a stable version of the software requiring minimal bug fixes.



Provide prompt, professional customer support.



Negotiate administrative hurdles together with customer.

...it can be purchased, installed and maintained in a corporate environment.

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 - **Multiscale** framework
 - **Technological** context
 - **Digital** environment
 - **Organizational** boundary conditions

Concluding thoughts

Industry provides materials modeling with:

1. **Opportunities:** a vast array of possible application
2. **Priorities:** achieving technological goals is essential
3. **Approaches:** getting the job done is what matters
4. **Limitations:** administrative hurdles are real



Thank you

Question and Answer Session



Dr. Volker Eyert

Materials Design



Dr. Jonathan Mueller

Volkswagen AG



MedeA Environment

- ▶ MedeA modules mentioned in today's webinar
<https://www.materialsdesign.com/property-modules>

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[MedeA HT Launchpad](#)

[MedeA VASP](#)

[MedeA UNCLE](#)

[MedeA Electronics](#)

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khollingsworth@materialsdesign.com



Question and Answer Session



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Questions about the webinar

Katherine Hollingsworth

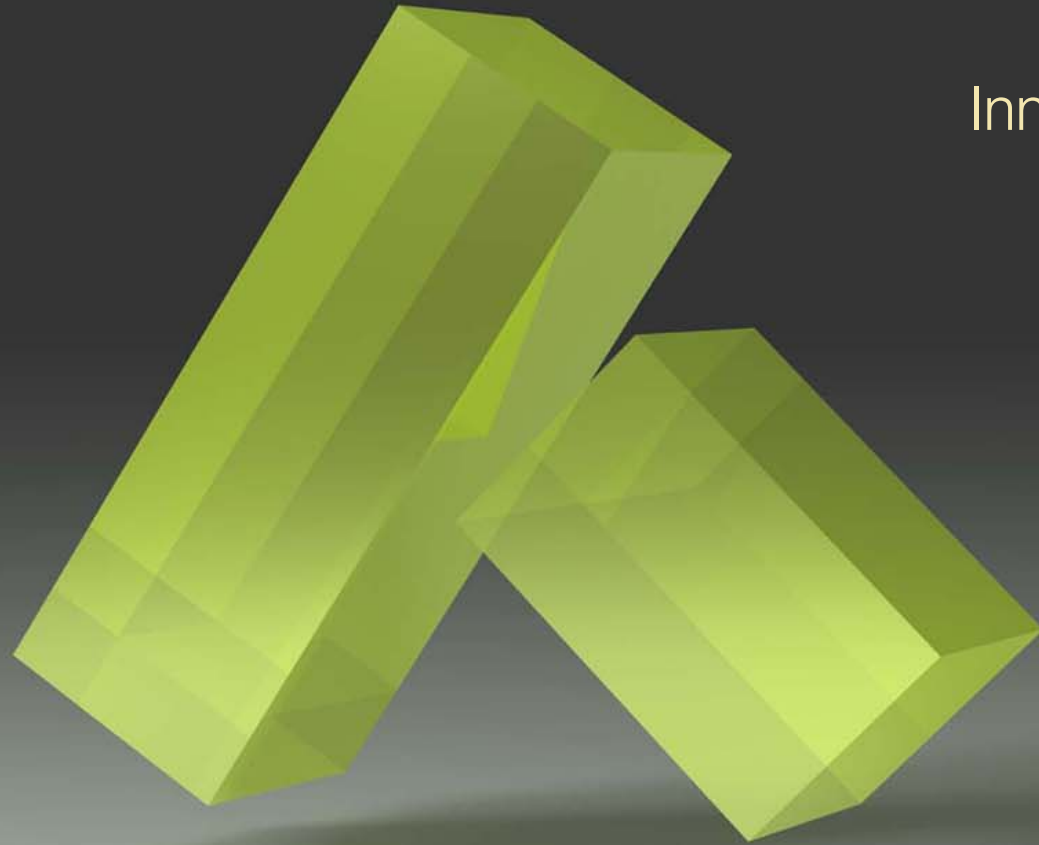
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Innovation by Simulation