



materials design

Li-Ion Batteries and Beyond: Driving Next-Generation Energy Storage with *MedeA*[®]


Training

Taylor Juran
Materials Design

Jan 2021



Materials Design Webinar Series

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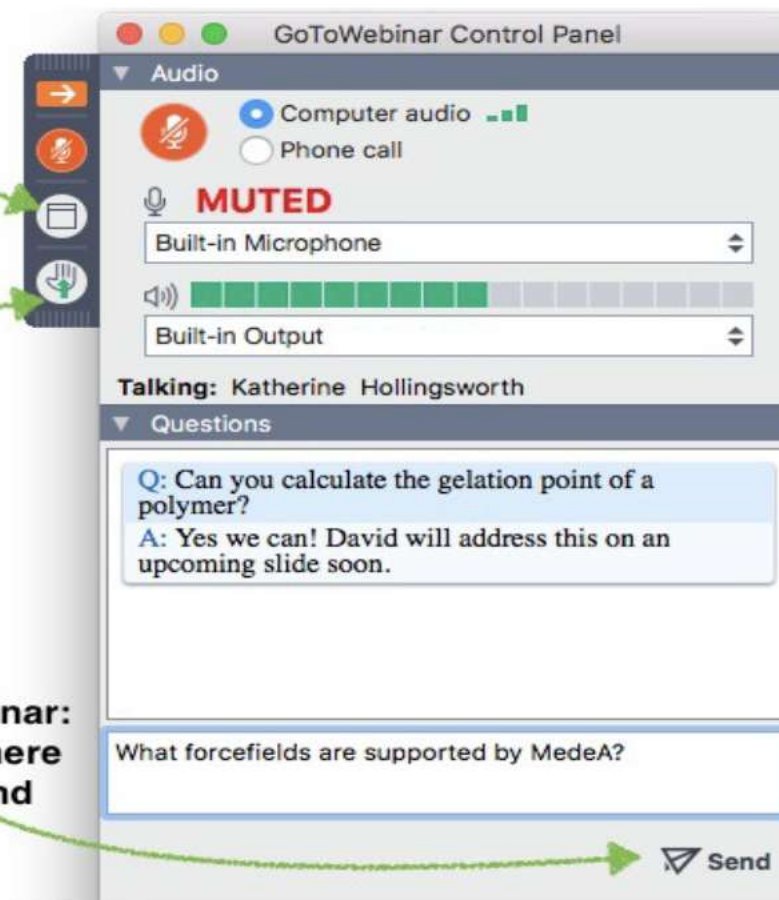
Materials Design Webinar Series

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Ray Shan

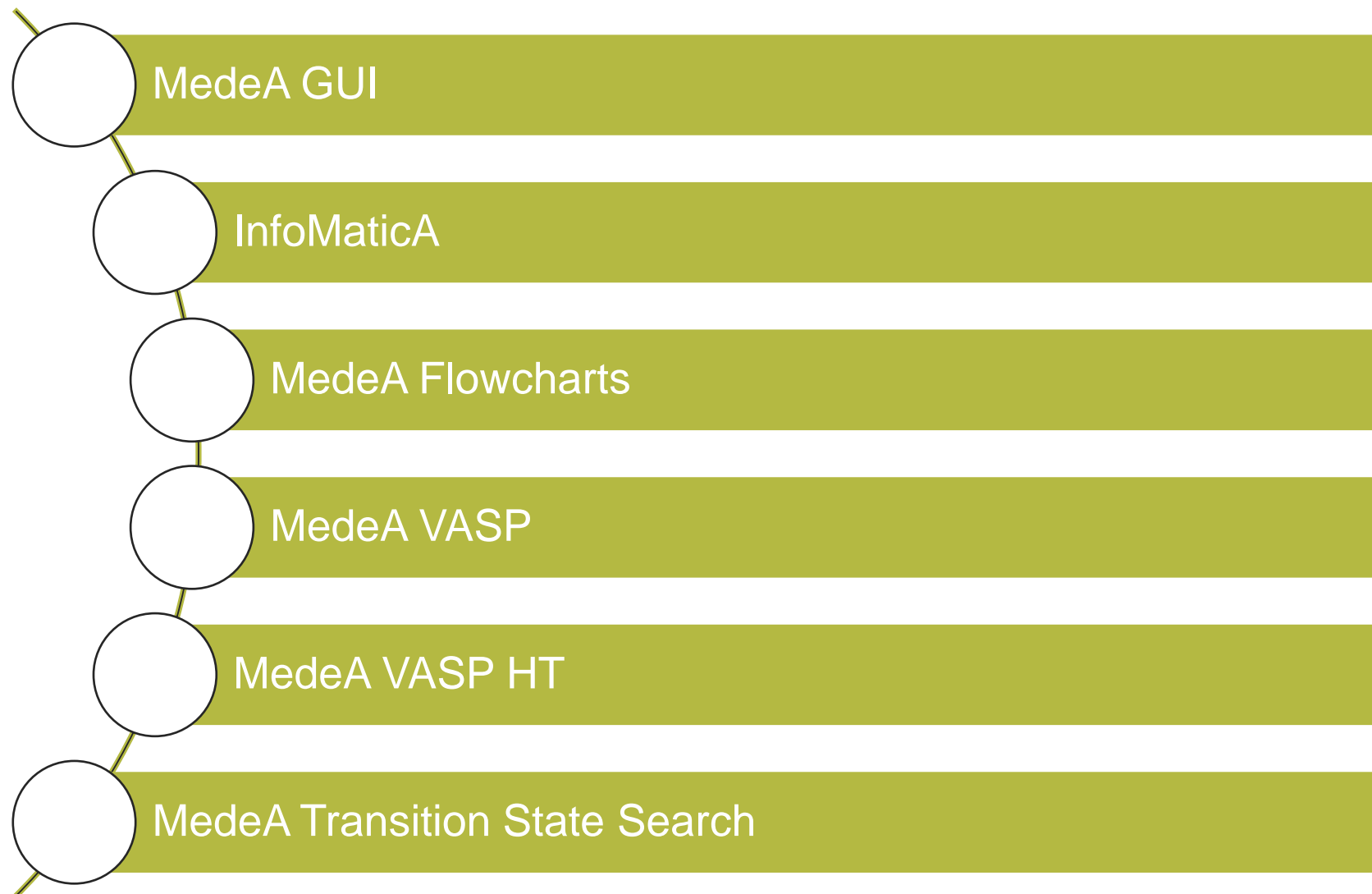
René Windiks

Taylor Juran
presenter

David Reith

Siwen Wang

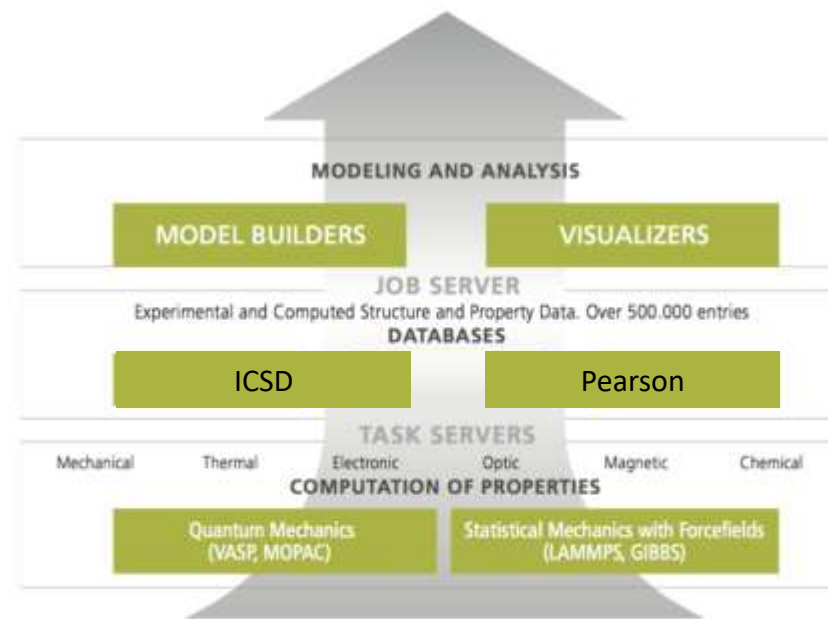
Outline



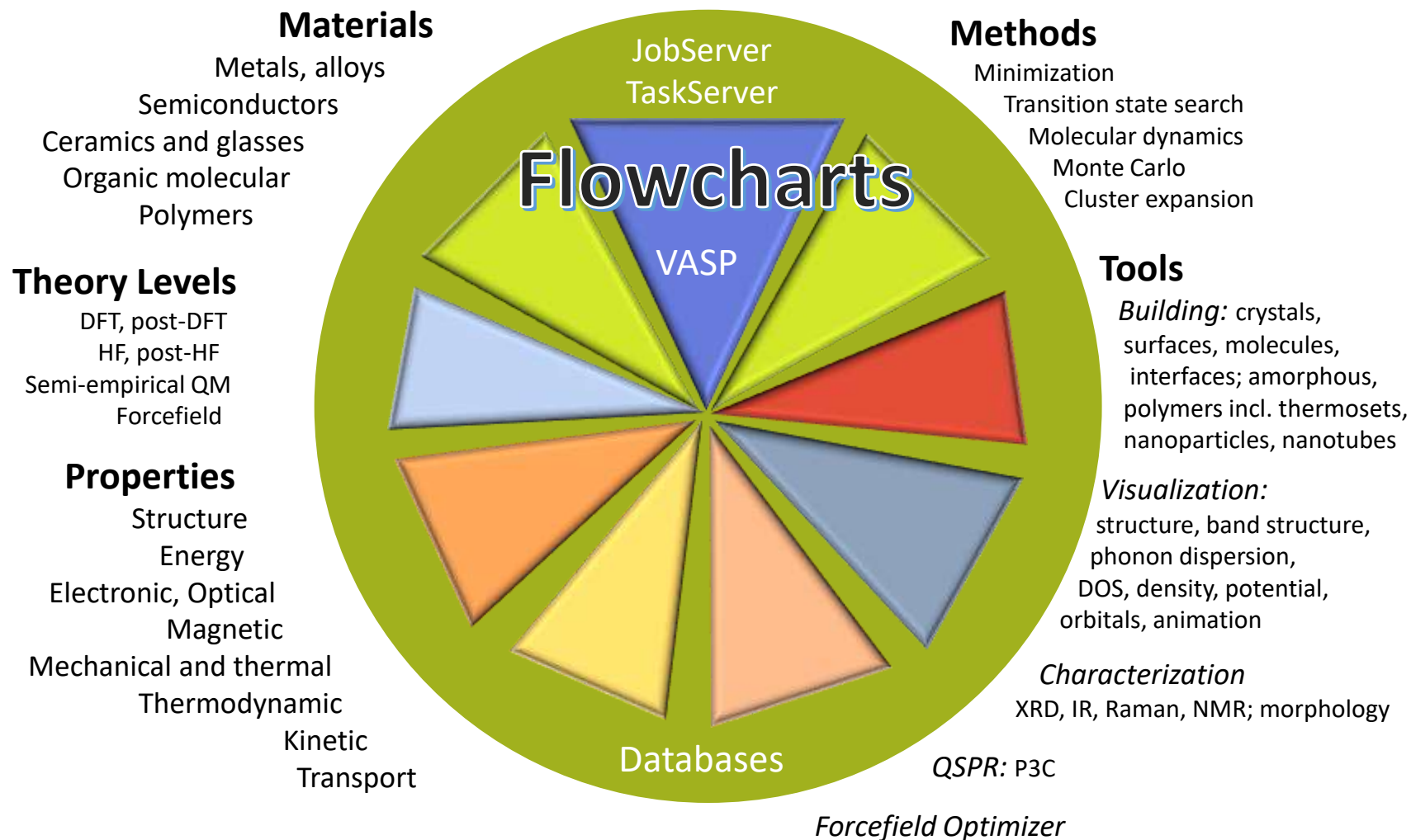
MedeA Software Environment

- **Engines**
 - VASP, GIBBS, LAMMPS, GAUSSIAN, MOPAC
- **Databases**
 - ICSD, Pauling, Pearson's, NIST, COD, InfoMaticA Query Engine, MPDS
- **Builders**
 - Crystals, nanoparticles, amorphous materials, interfaces, molecules, polymers, conformers, thermosets, docking
- **Forcefields**
 - Forcefields bundle, Forcefield Optimizer
- **Property Modules**
 - MT, TSS, Phonon, Electronics, UNCLE, LAMMPS (Diffusion, Thermal Conductivity, Viscosity, CED, Surface Tension), P3C,

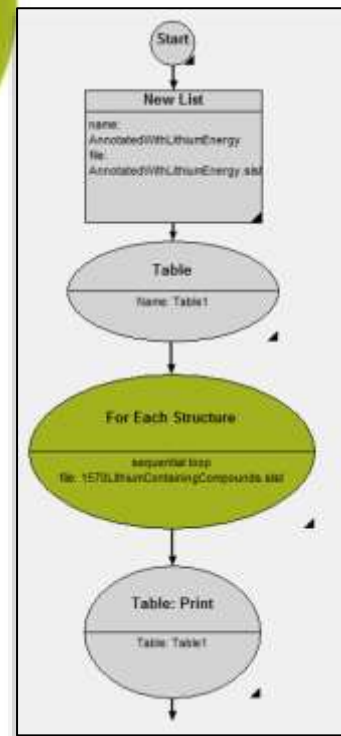
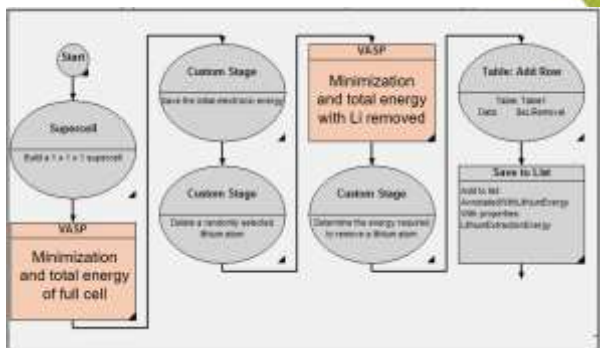
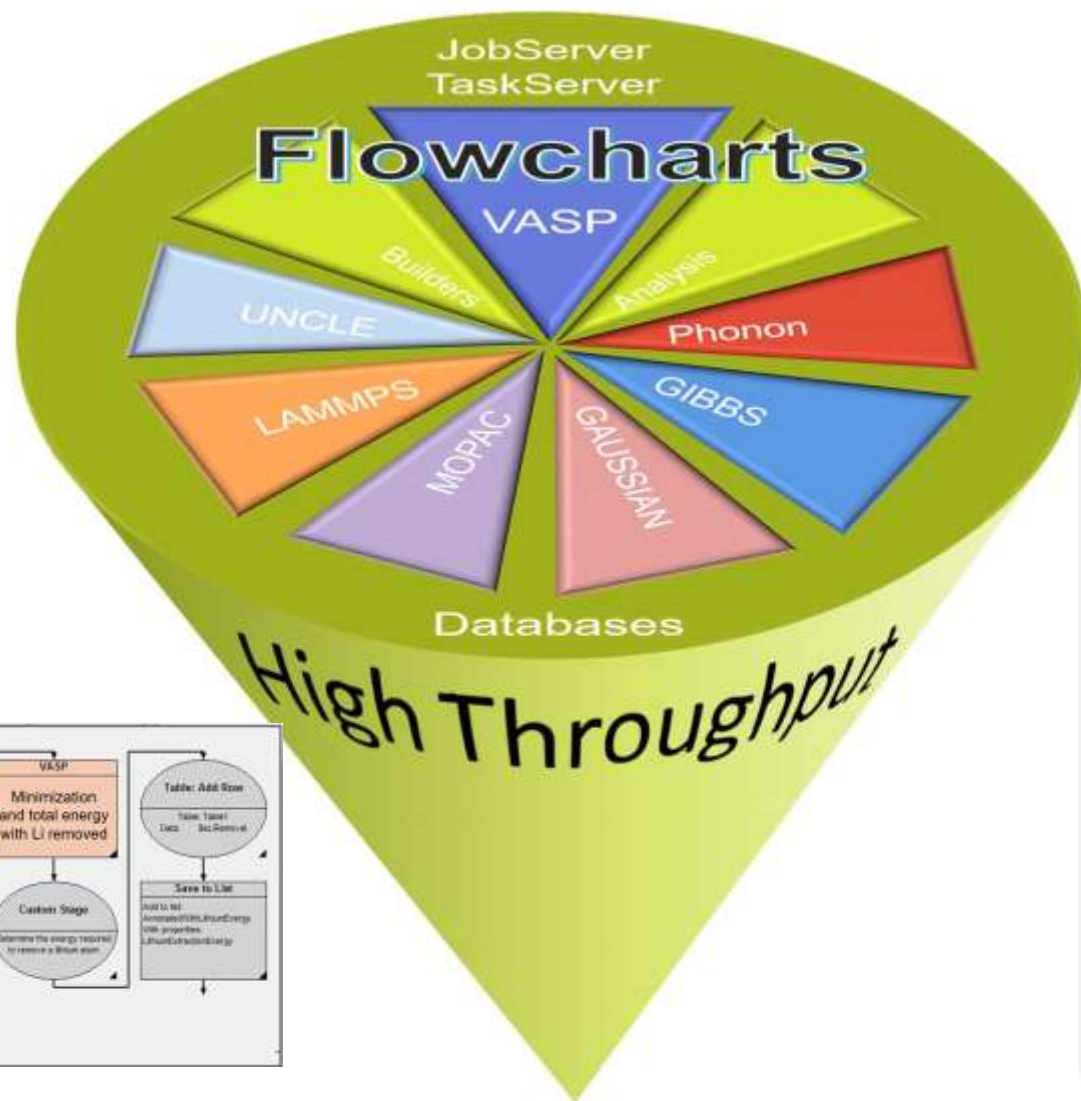
- **High Throughput**
 - HT-Launchpad, HT-Descriptors, HT-correlation
- **Analysis**
 - Broad range of analysis tools
- **JobServer & TaskServer**



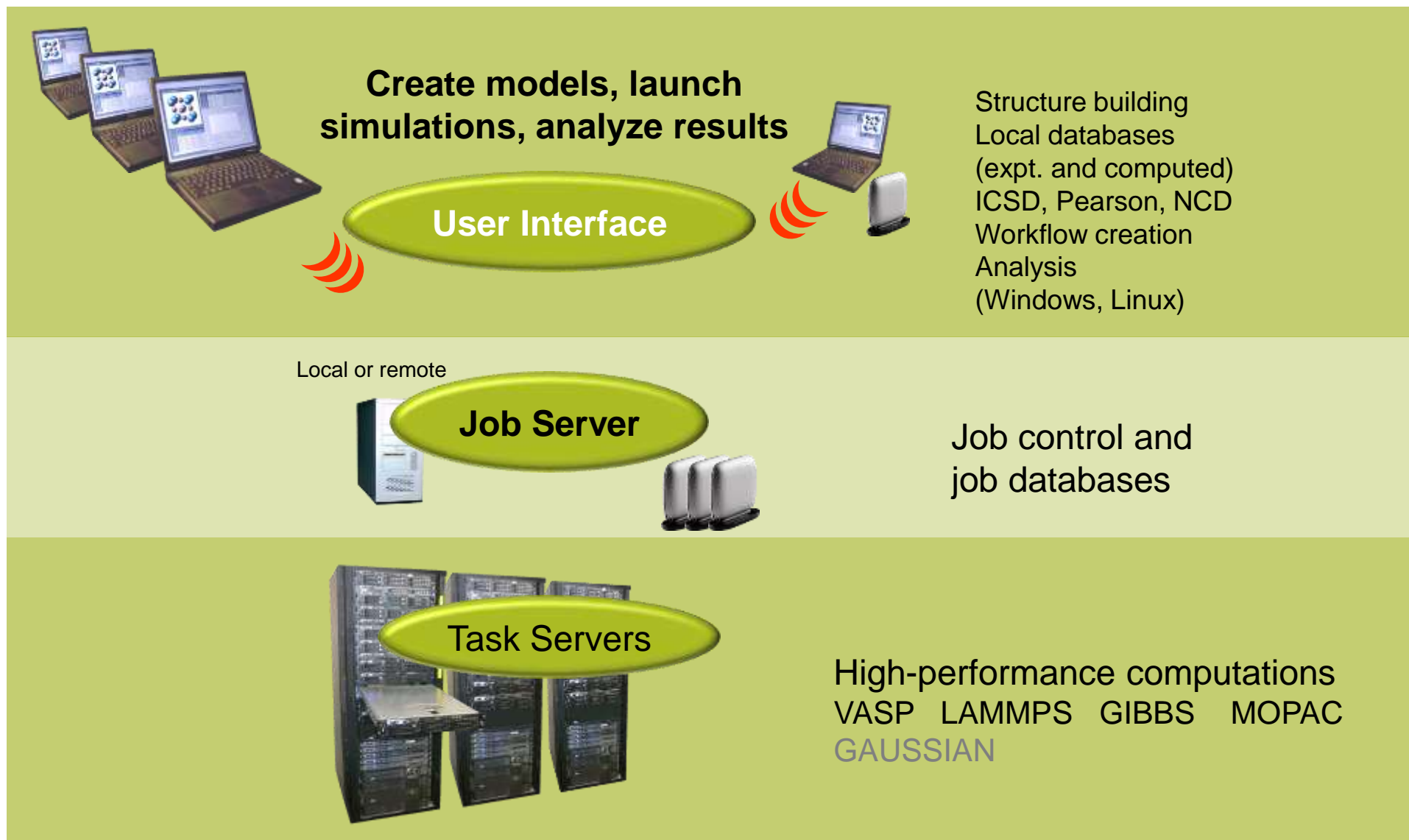
MedeA Software Environment



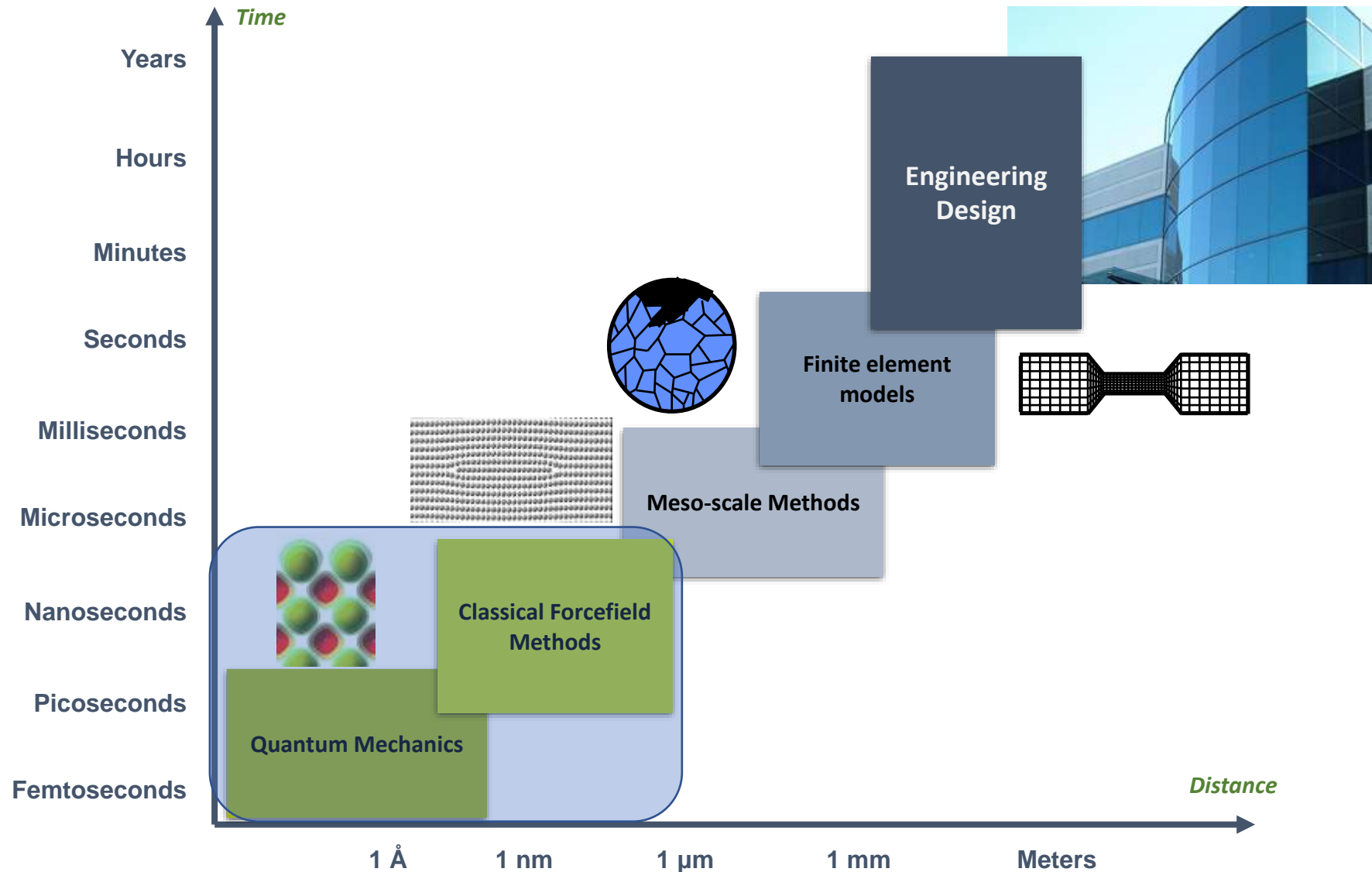
MedeA Software Environment



MedeA 3-Tier Architecture



Overview of Materials Simulation Methods



Materials Properties from *MedeA*

Structural properties

- Molecular structures
- Crystal structures
- Surface structures
- Structure around defects
- Adsorption geometries
- Structures of interfaces
- Liquids and amorphous systems

Thermo-Mechanical properties

- Density
- Elastic moduli
- Thermal expansion coefficients
- Fracture

Thermodynamic properties

- ΔU , ΔH , ΔS , ΔG , heat capacity
- Binding energies
- Solubility
- Melting temperature
- Vapor pressure
- Miscibility
- Phase diagrams
- Surface tension

Chemical properties

- Chemical reaction mechanisms and rates
- Reactivity on surfaces
- Solid-solid reactions
- Photochemical reactions

Transport properties

- Mass diffusion coefficient
- Permeability
- Thermal conductivity
- Viscosity
- Electrical conductivity

Electronic, optical, and magnetic properties

- Electron density distribution - electrical moments
- Polarizabilities, hyperpolarizabilities
- Optical spectra
- Dielectric properties
- Piezoelectric properties
- Electrostatic potential
- Spin density distribution, magnetic moments
- Energy band structure - metal, semiconductor, insulator
- Band gaps, band offsets at hetero-junctions
- Ionization energies and electron affinities
- Work function

Conclusion: What we have learned

- How the MedeA software environment works
- About the MedeA 3-tier architecture
- Locate intercalation sites within a cathode
- Perform VASP HT calculations on intercalated cathodes
- Calculate and view the DOS
- MedeA Transition State Search to view diffusion barriers

Upcoming Webinar

Machine Learning Meets Quantum Chemistry: Using Theory, Data, and Experiments to Design Catalysts

Presented by Dr. Siwen Wang

February 2nd 3rd, 4th

Register www.materialsdesign.com/webinars



Online Training and Demo

Machine Learning Meets Quantum Chemistry:
Using Theory, Data, and Experiments to
Design Catalysts

Thursday, February 11, 2021

USA/EUROPE:


10:00 am PST/1:00 pm EST

7:00 pm CEST

Register for the training:

<https://www.materialsdesign.com/webinar-register/Machine-Learning-Quantum%20Chemistry-Catalysts>

*Training open to everyone



Online Training and Demo:
Machine Learning Meets
Quantum Chemistry:
Using Theory, Data, and
Experiments to Design
Catalysts

Li-Ion Batteries and Beyond

- **MedeA modules mentioned in today's training**
 - <https://www.materialsdesign.com/compute-engines>
 - <https://www.materialsdesign.com/analysis-tools>
 - [*MedeA Environment*](#)
 - [*MedeA VASP*](#)
 - [*MedeA HT*](#)
 - [*MedeA Transition State Search \(TSS\)*](#)
- **Webinar: Live and Recorded**
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- **Publications**
 - <https://www.materialsdesign.com/Publications>
- **Application Notes**
 - <https://www.materialsdesign.com/application-notes>
- **For questions or comments contact**
 - Katherine Hollingsworth
 - khollingsworth@materialsdesign.com

Question and Answer Session



Dr. René Windiks

Materials Design



Dr. Taylor Juran

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Questions about Materials Design Trainings

Materials Design Support Team

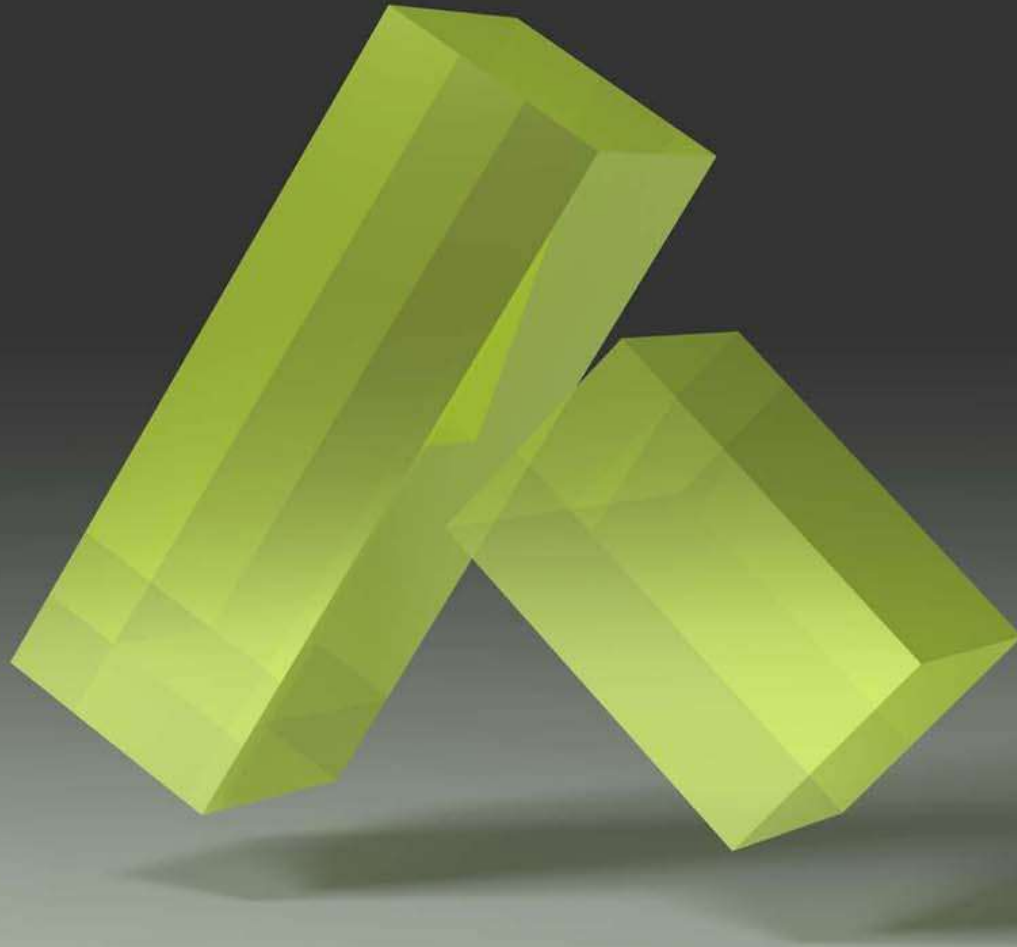
support@materialsdesign.com



materials design

info@materialsdesign.com

www.materialsdesign.com



Medea

Innovation by Simulation