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# Training: Orbital Level Understanding of Adsorbate-Surface Interactions in Catalysis

Siwen Wang  
Materials Design

February 2021



# Materials Design Webinar Series

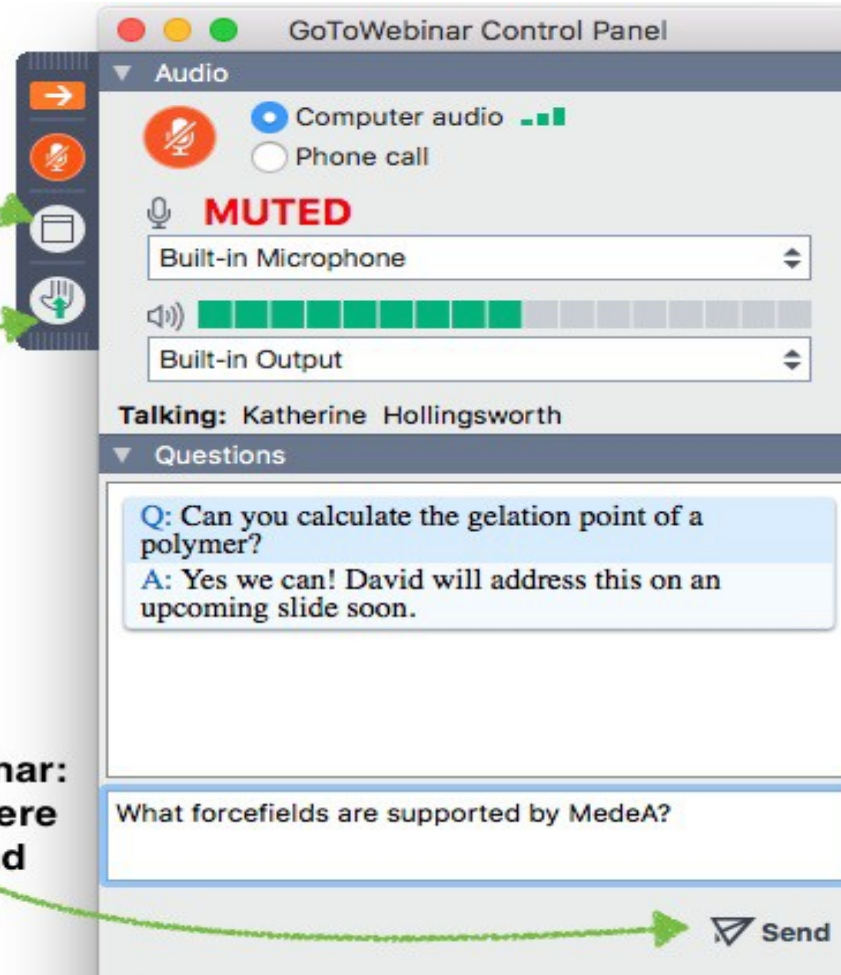
- ▶ We will be recording this training
  
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  - <http://www.materialsdesign.com/webinars/recorded>
  - The recording and training will be under the related webinar: Machine Learning Meets Quantum Chemistry Using Theory Data and Experiments to Design Catalysts
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# Please Ask Questions!

**Use the raise hand icon to bring attention to your question**

**full screen**  
**during discussion:**

**any time during webinar:  
type your question here  
and then press Send**



The screenshot shows the GoToWebinar Control Panel interface. It includes a sidebar with icons for full screen, mute, and raise hand. The main panel displays audio settings (Computer audio selected, muted), a microphone dropdown menu, a volume slider, and an output dropdown menu. Below this, it shows the current speaker (Katherine Hollingsworth) and a 'Questions' section. The questions section contains a question: 'Q: Can you calculate the gelation point of a polymer?' and an answer: 'A: Yes we can! David will address this on an upcoming slide soon.' At the bottom, there is a text input field with the question 'What forcefields are supported by Medea?' and a 'Send' button.



# Speakers

***Katherine Hollingsworth***

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***Siwen Wang***

*swang@materialsdesign.com*

***Taylor Juran***

*tjuran@materialsdesign.com*



***David Reith***

***René Windiks***

***Siwen Wang***

***Taylor Juran***

***Ray Shan***



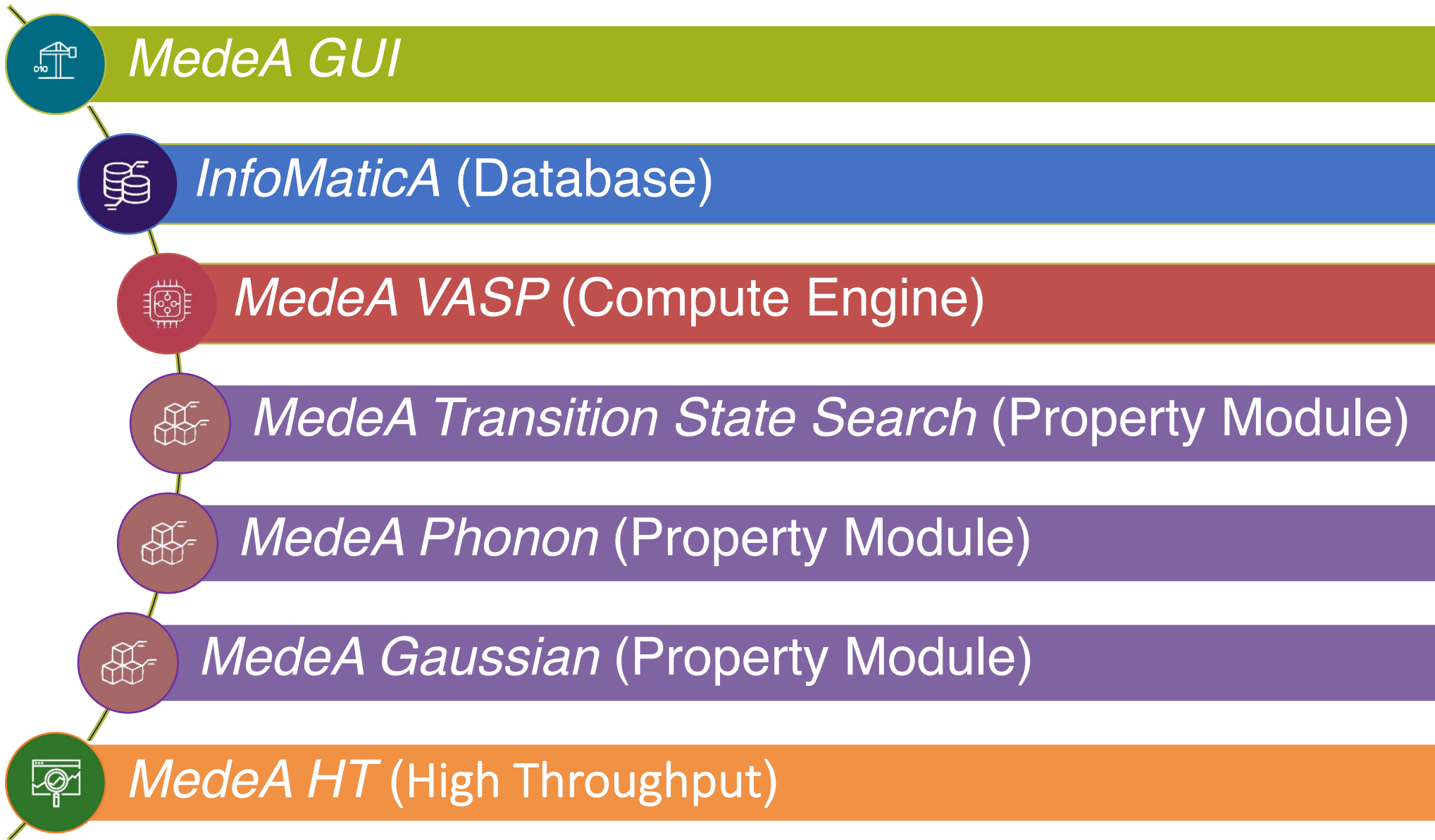
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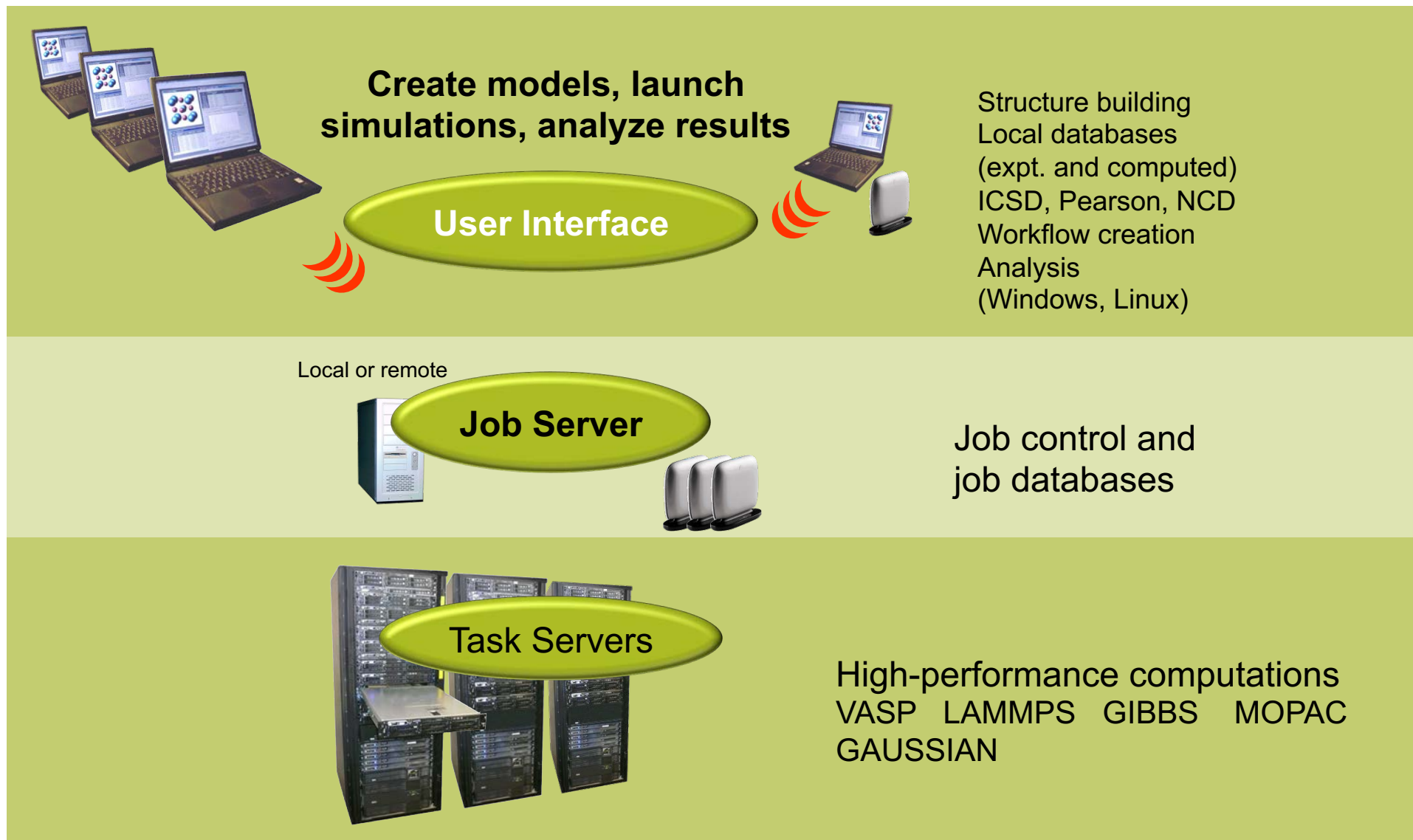
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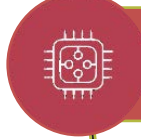
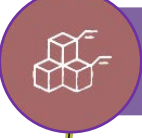
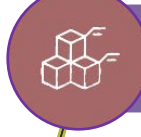
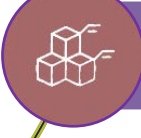

# Outline



# MedeA Overview



# Conclusion

-  Had an overview of *MedeA GUI*
-  Extracted structure from *InfoMaticA*
-  Learnt how to do *VASP* calculations
-  Calculated energy barrier using *MedeA TSS*
-  Calculated Gibbs free energy using *MedeA Phonon*
-  Calculated Gibbs free energy using *MedeA Gaussian*
-  Performed high-throughput calculations using *MedeA HT*



# Upcoming Webinar

Materials Constitution Data in MSI Eureka –  
Fundamentals for Efficient R&D

Register:

[www.materialsdesign.com/webinars](http://www.materialsdesign.com/webinars)

March 4<sup>th</sup>, 2021



# Design Catalysts

- ▶ MedeA modules mentioned today
  - <https://www.materialsdesign.com/compute-engines>
  - <https://www.materialsdesign.com/analysis-tools>
  - [MedeA Environment](#)
  - [MedeA VASP](#)
  - [MedeA HT](#)
  - [MedeA Phonon](#)
  - [MedeA Gaussian](#)
  - [MedeA Transition State Search \(TSS\)](#)

- ▶ Webinar: Live and Recorded
  - <https://www.materialsdesign.com/webinars>
- ▶ Publications
  - <https://www.materialsdesign.com/Publications>
- ▶ Application Notes
  - <https://www.materialsdesign.com/application-notes>
- ▶ For questions or comments contact:  
  
Katherine Hollingsworth  
[khollingsworth@materialsdesign.com](mailto:khollingsworth@materialsdesign.com)

# Question and Answer Session



***Dr. Siwen Wang***

*Materials Design*



***Dr. Taylor Juran***

*Materials Design*

# Questions about Materials Design Trainings

***Materials Design Support Team***

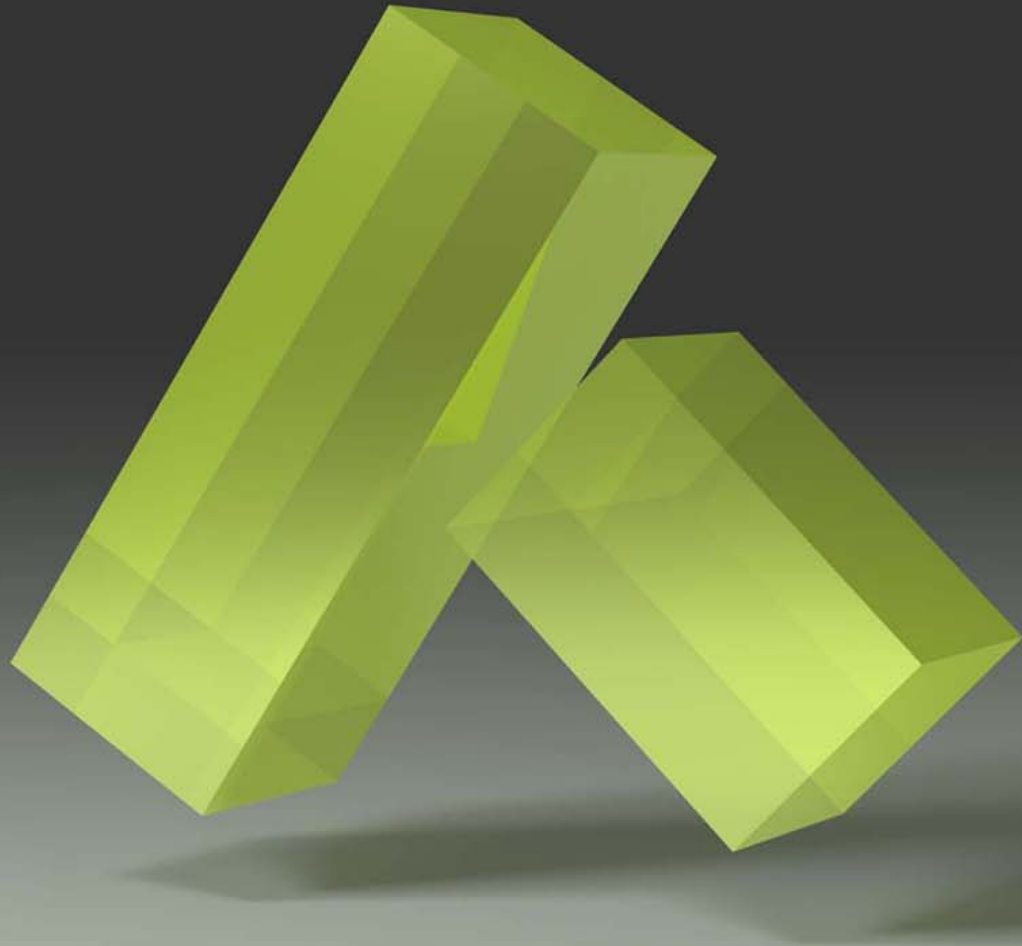
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# *Medea*

Innovation by Simulation