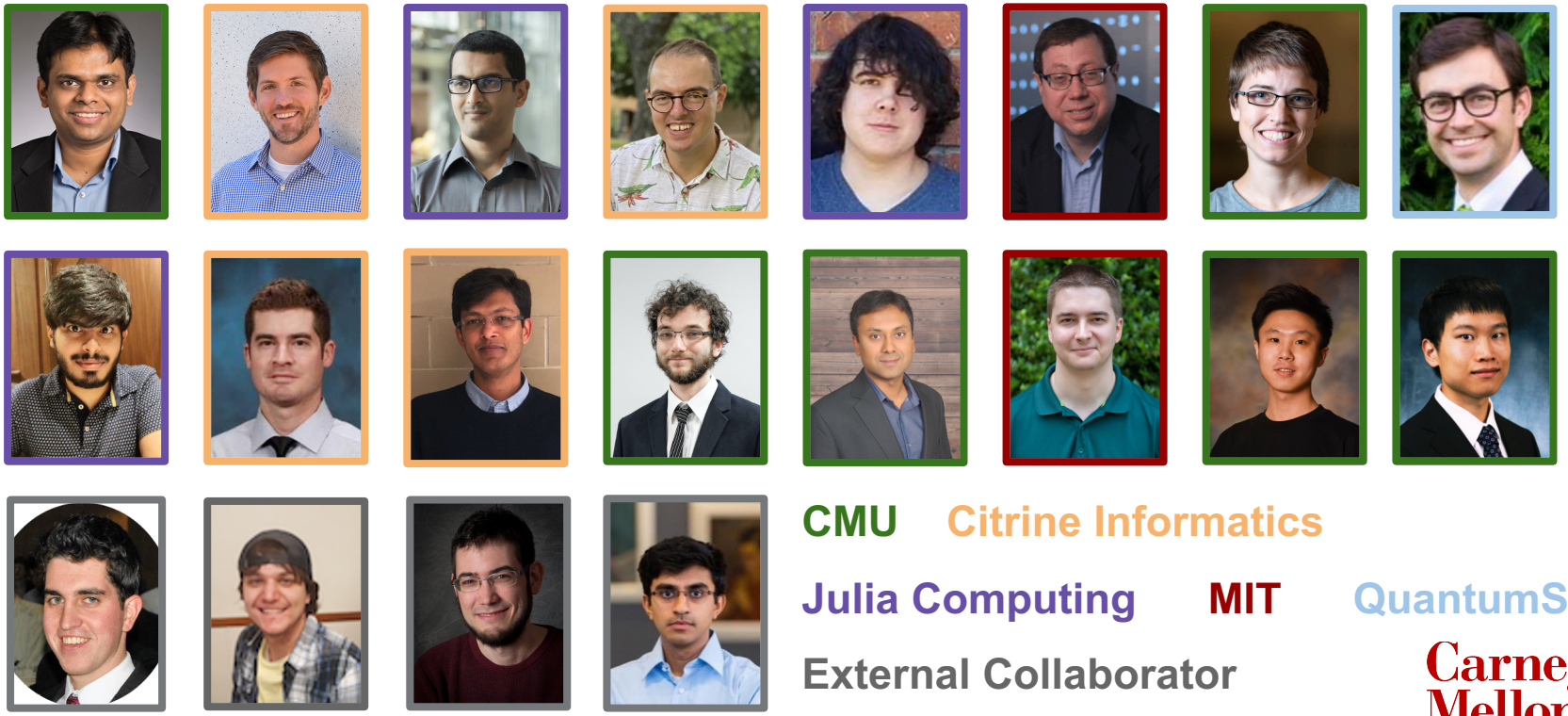
Carnegie Mellon University

High-fidelity Accelerated Design of High-performance Electrochemical Systems

Rachel Kurchin

Postdoctoral Fellow, Carnegie Mellon University

Our Team



CMU Citrine Informatics

Julia Computing MIT QuantumScape

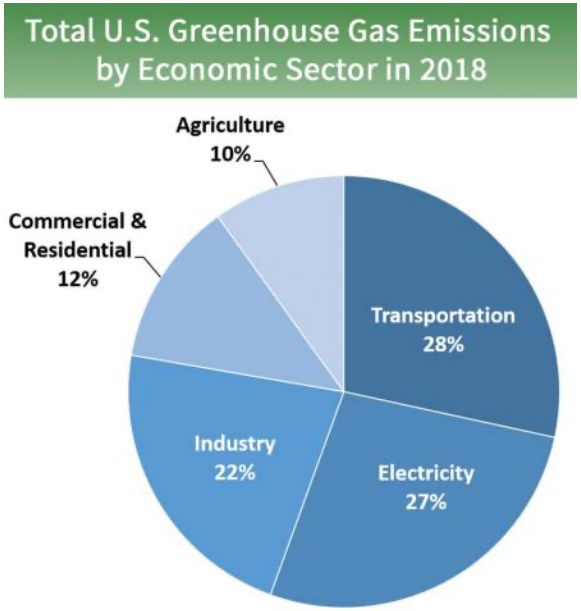
External Collaborator

Carnegie Mellon University

https://www.cmu.edu/aced/

Electrification is key to addressing the climate crisis

- Renewable electricity sources (e.g. photovoltaics, wind) are critical, but insufficient
- Electrochemical devices provide ways to **store electricity** and also to **electrify industries** that still rely on fossil fuels
- We are developing a *generalizable workflow* for significantly faster discovery of new electrochemical materials and systems than was previously possible
- Two specific case studies
    - Electrochemical ammonia production (fertilizers)
    - Lithium-metal batteries (transportation+)



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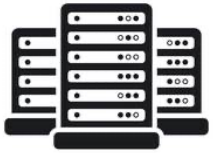
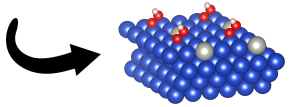
https://www.epa.gov

State-of-the-Art





Generate structures

First-principles simulation (DFT, quantum chemistry, …)

Materials properties

ODE/DAE solvers (MKM, device model, …)

Design space search: select new candidate

Device performance prediction

success!

Experimental testing

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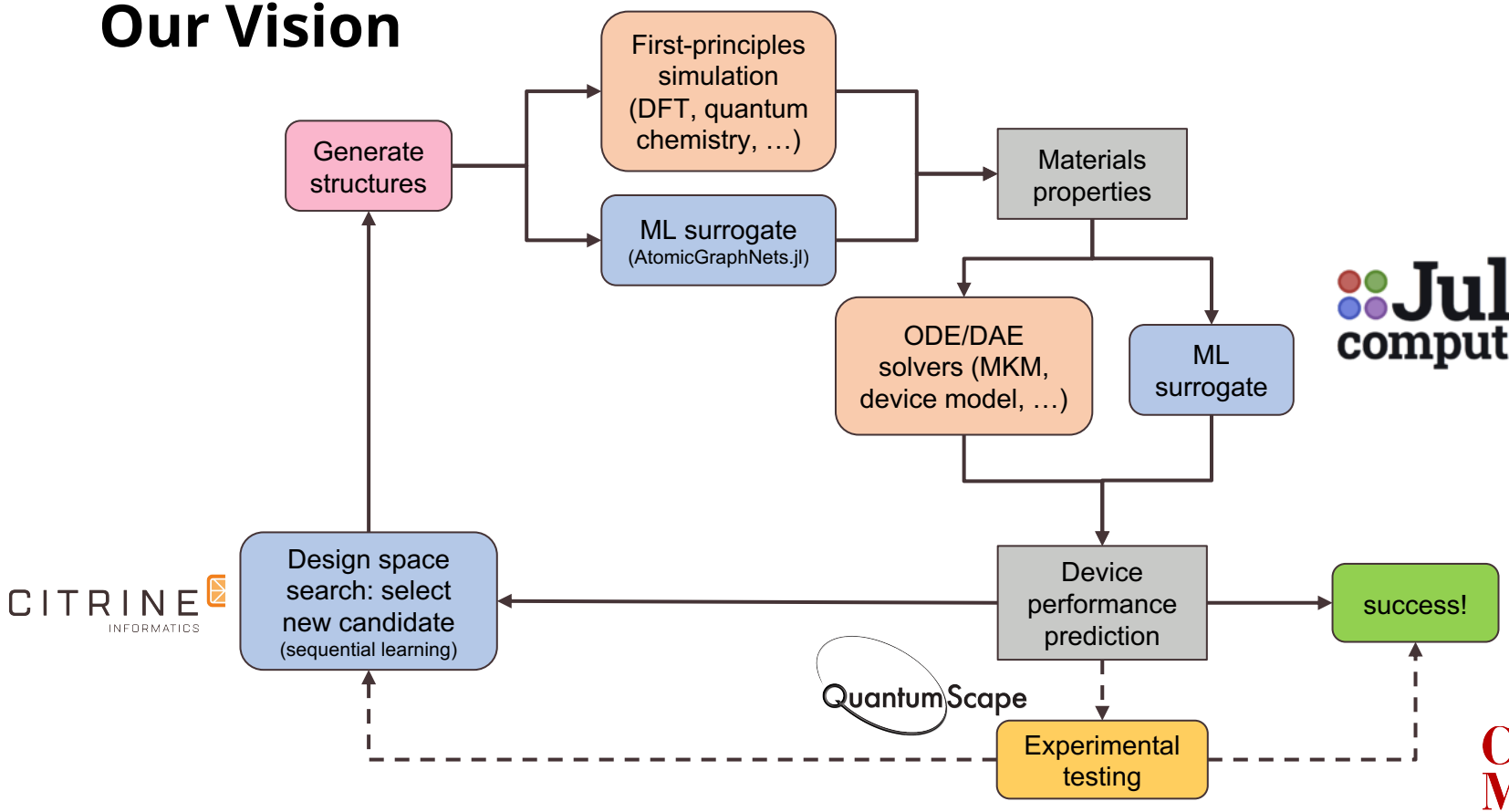
Our Vision


First-principles simulation (DFT, quantum chemistry, …)
Generate structures
ML surrogate (AtomicGraphNets.jl)
Materials properties
ODE/DAE solvers (MKM, device model, …)
ML surrogate
Julia computing
CITRINE INFORMATICS
Design space search: select new candidate (sequential learning)
Device performance prediction
success!
QuantumScape
Experimental testing
Carnegie Mellon University

Acknowledgements / Contact Information

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https://www.cmu.edu/aced

https://www.github.com/aced-differentiate

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