The **MA**terials **S**imulation **T**oolkit for Defect and Diffusion Calculations

Tam Mayeshiba, Henry Wu, Zhewen Song, Ben Afflerbach, Professor Dane Morgan

University of Wisconsin-Madison

NIST/CHiMaD Data Workshop, Evanston, IL
May 2, 2016

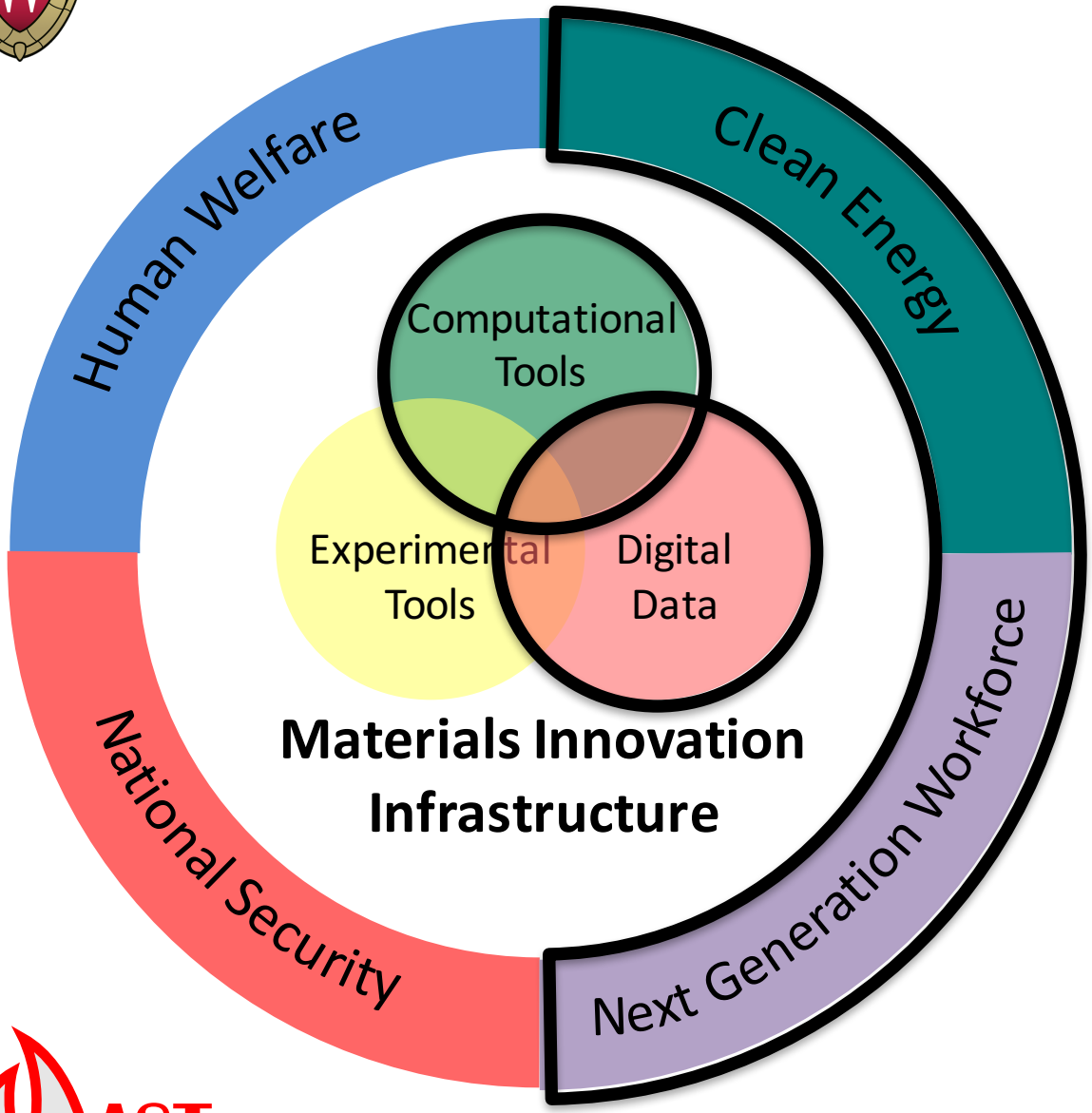
http://pythonhosted.org/MAST

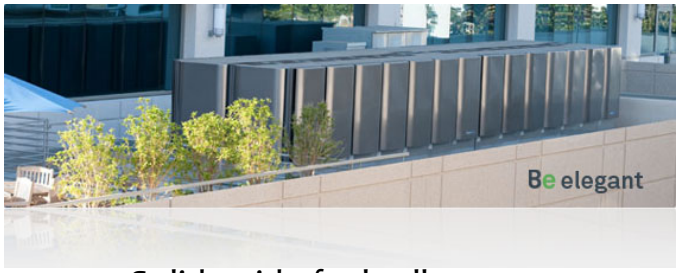
Computational Materials Group

NSF

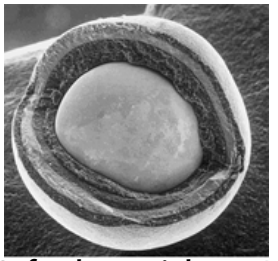
WISCONSIN
UNIVERSITY OF WISCONSIN–MADISON

MAST's role in the Materials Genome Initiative

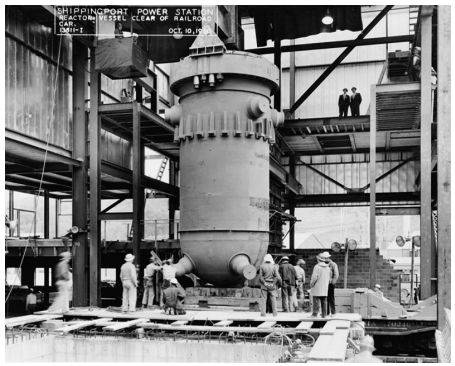




Solid oxide fuel cell server, bloomenergy.com



TRISO fuel particle, US DOE



Reactor pressure vessel, US DOE

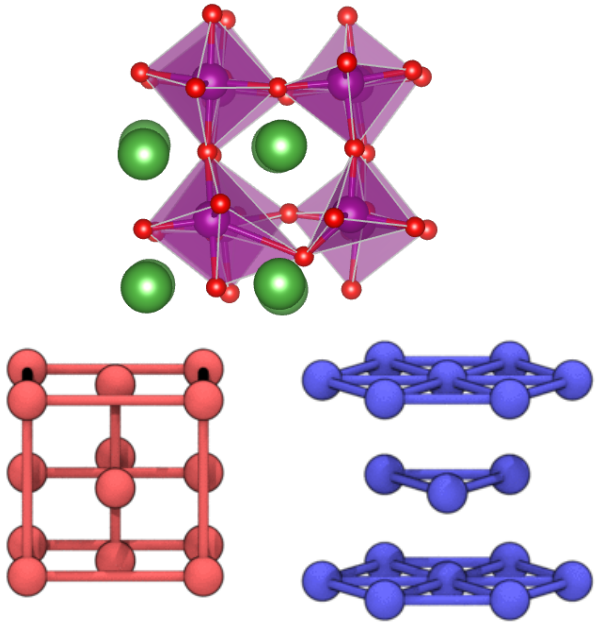
MAST
MAterials Simulation Toolkit

MGI image retouched from https://www.whitehouse.gov/mgi

What is MAST?

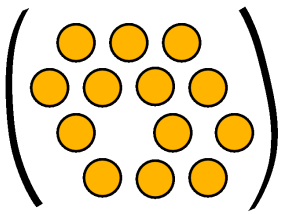
python™ pymatgen

MAterials Simulation Toolkit

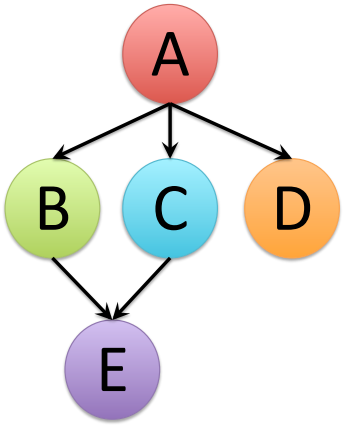


Motivated by materials science: defects and diffusion

b-initio VASP ackage ienna imulation



Created for simulations (materials calculations)



$$D = A\exp\left(\frac{-Q}{kT}\right)$$

Workflow manager and post-processor

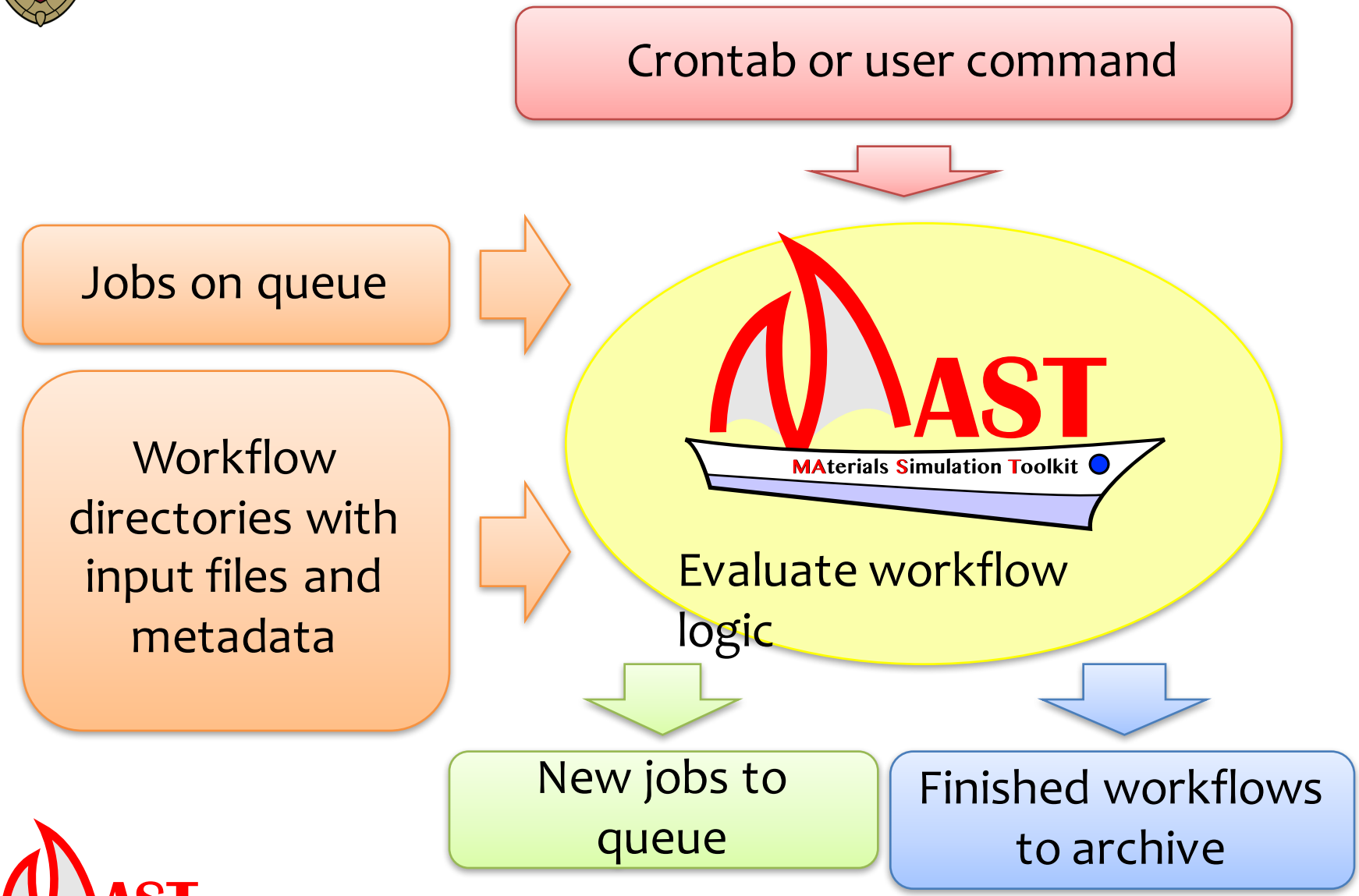
MAST MAterials Simulation Toolkit

Outline: Advantages of MAST

- Automatically manage workflows
  - MAST workflow management overview
  - Setting up a simple defect and diffusion workflow
  - Actual diffusion workflow schematic
  - Modify a workflow at any time
  - Manage workflows on various clusters
- Iterate easily over calculation system features
- Store and share workflow knowledge (VASP, diffusion, defects)
- Produce highly organized, consistently calculated data
  - Dilute solute diffusion
  - Scale examples of MAST-generated data
  - Storing MAST-generated data

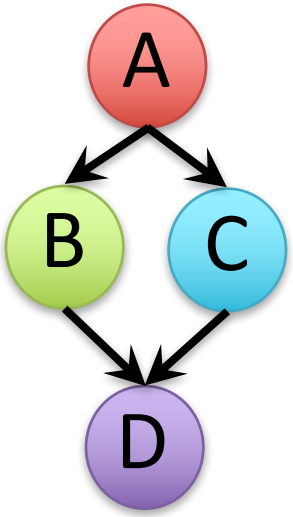
MAST
MAterials Simulation Toolkit

MAST workflow management overview



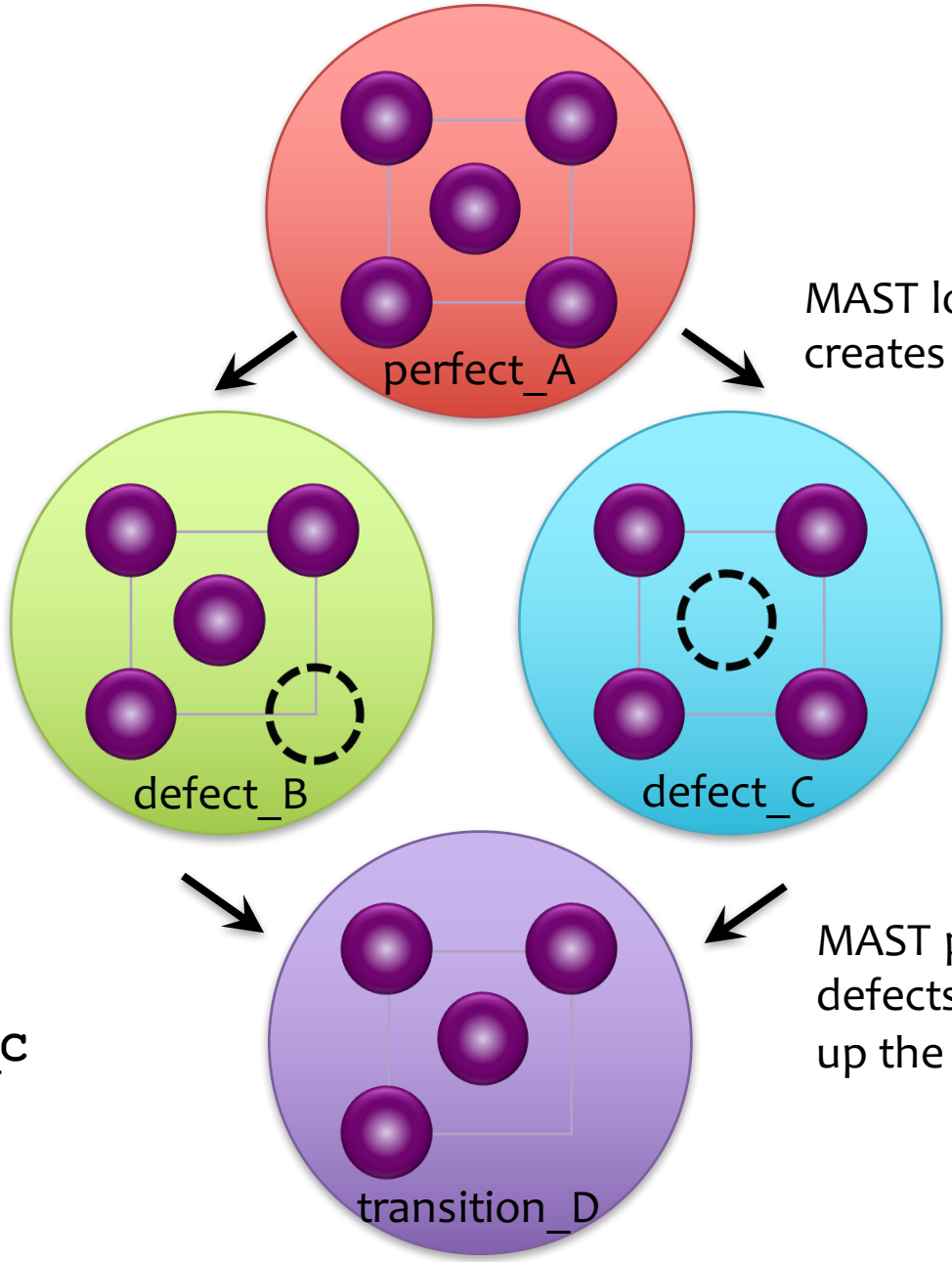
Setting up a simple defect and diffusion workflow

Directed Acyclic Graph (DAG) structure



How the DAG appears in the MAST input file:

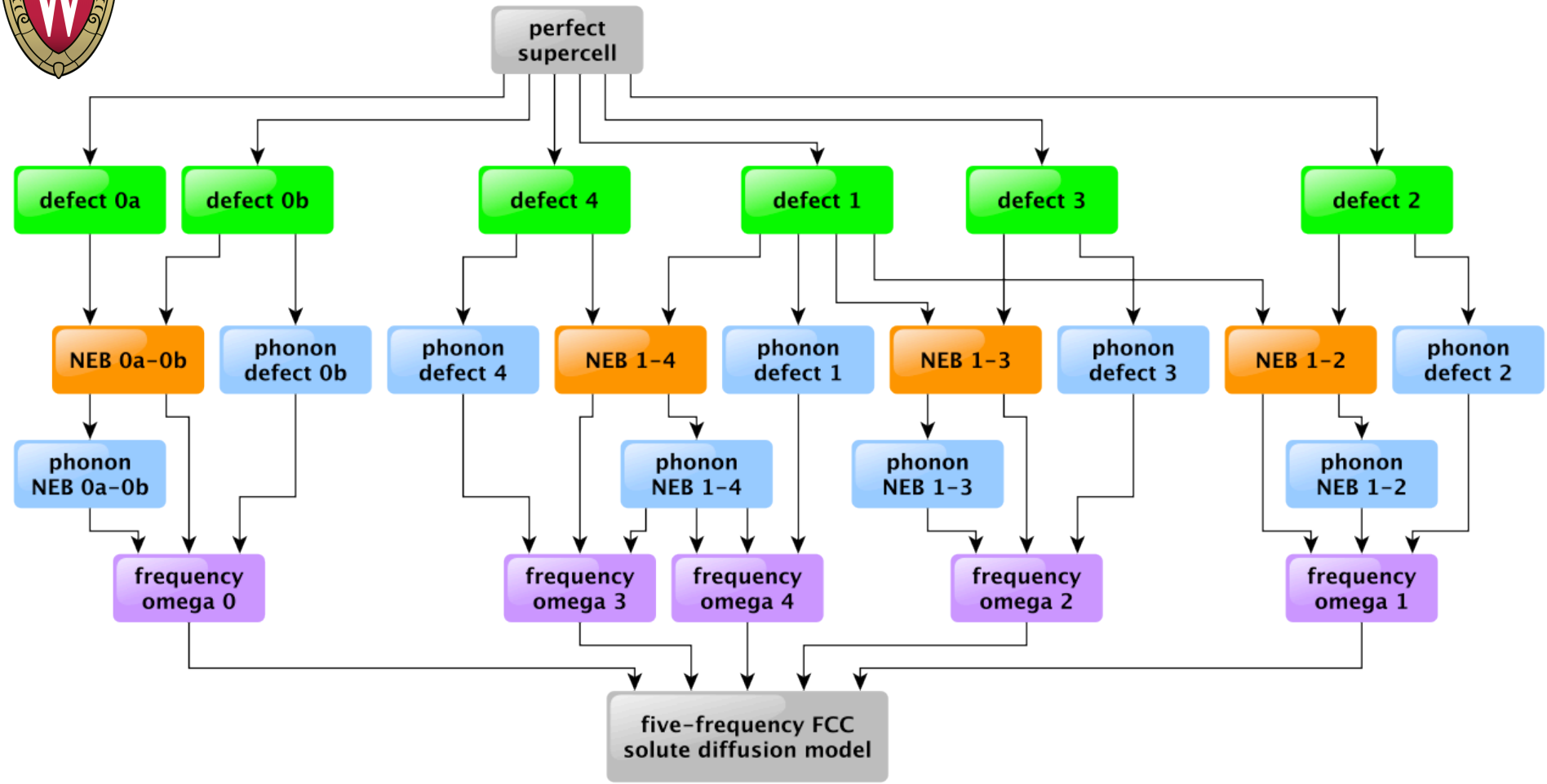
```
perfect_A
     defect_B
     defect_C
defect_B, defect_C
     transition_D
```



MAST locates and creates defects

MAST pairs up defects and sets up the path

Actual diffusion workflow schematic



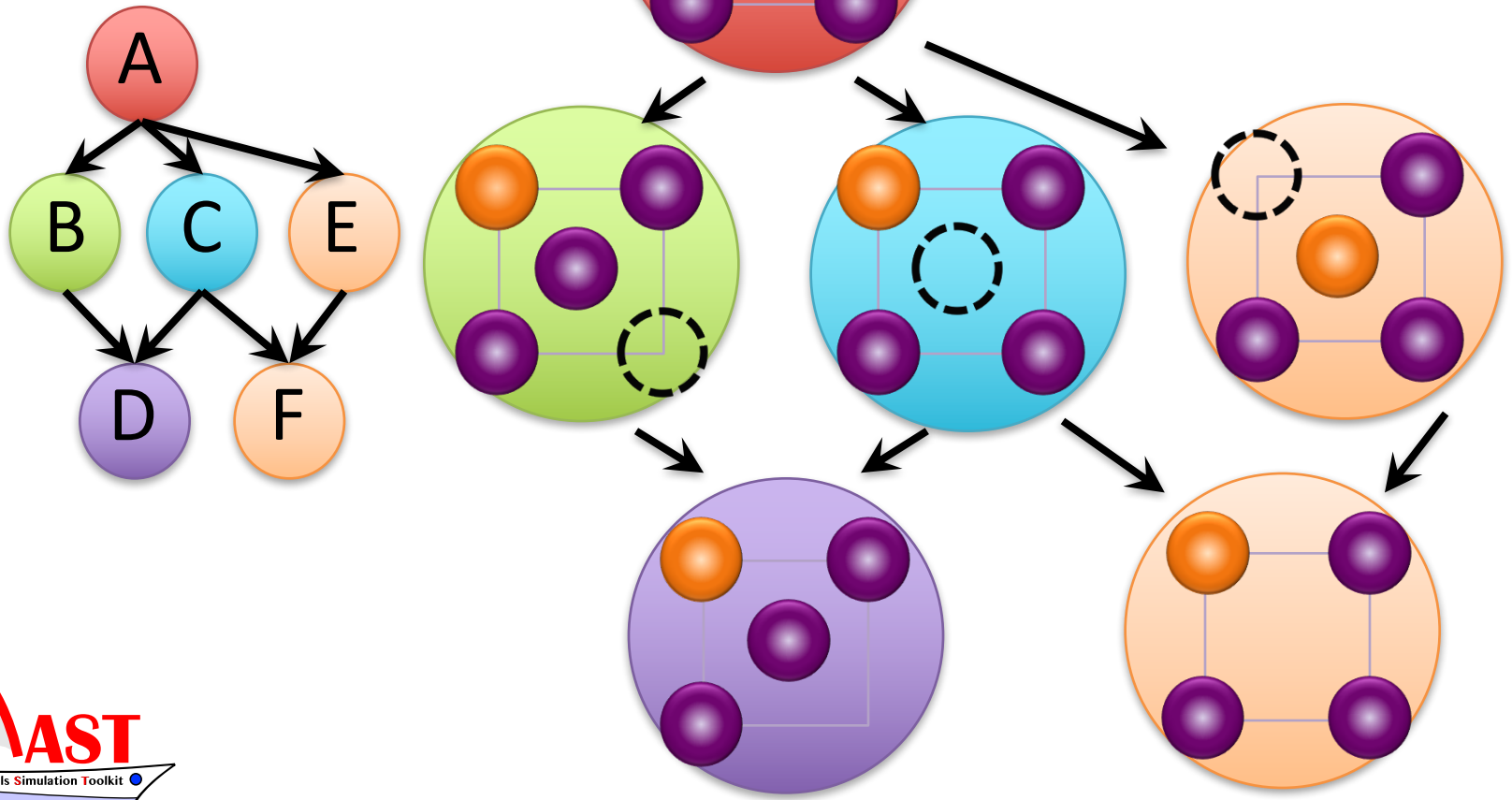
- 32 steps (not all steps are shown)
- Managing one case by hand is time-consuming and error prone
- Managing many workflows for many host-solute combinations by hand would be even worse => use MAST instead

MAST
MAterials Simulation Toolkit

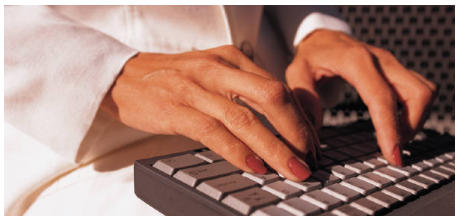
Modify a workflow at any time

Missed a step? Add branches to workflows mid-completion and rerun

Example: Forgot the solute hop! Add a new branch with a defect calculation and a path calculation.



Manage workflows on various clusters



External cluster

External cluster

External cluster

Local cluster

slurm workload manager

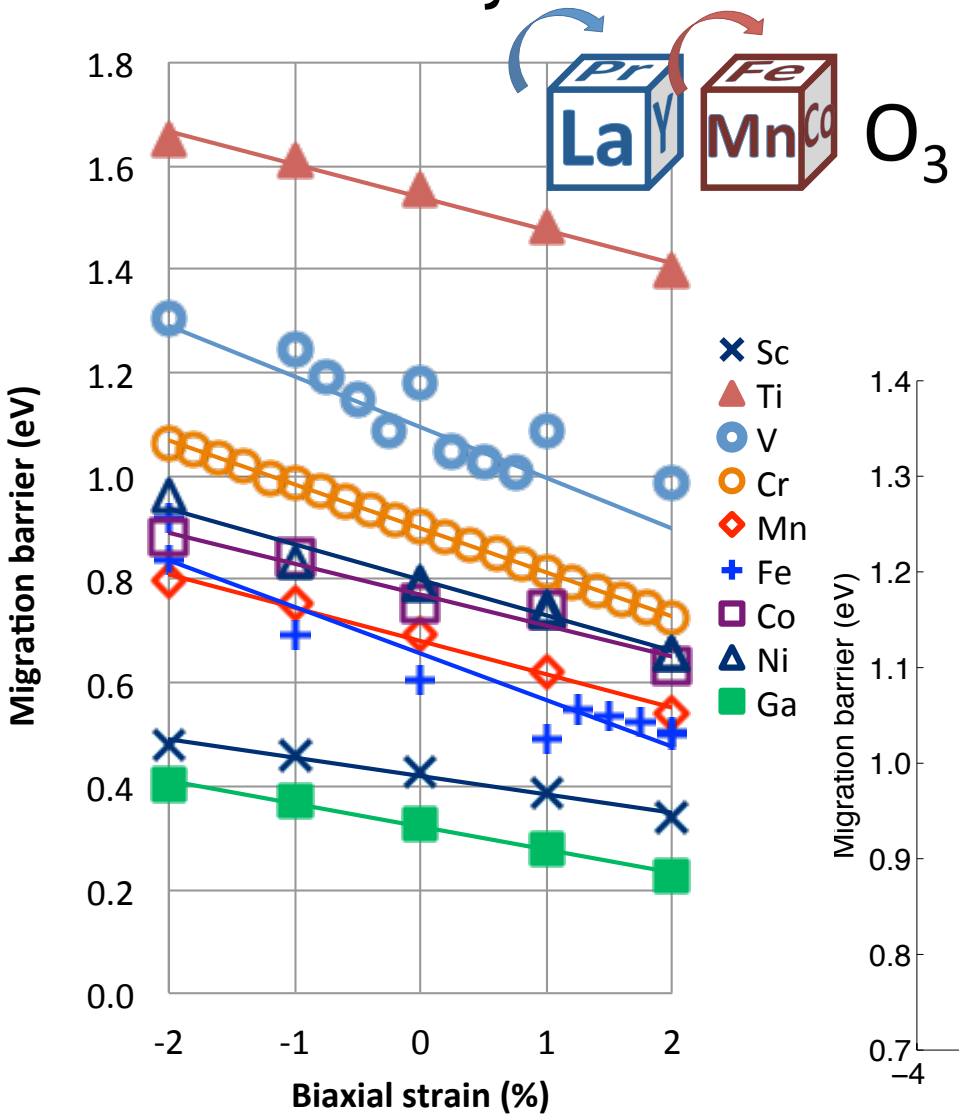
PBS/Torque

grid engine

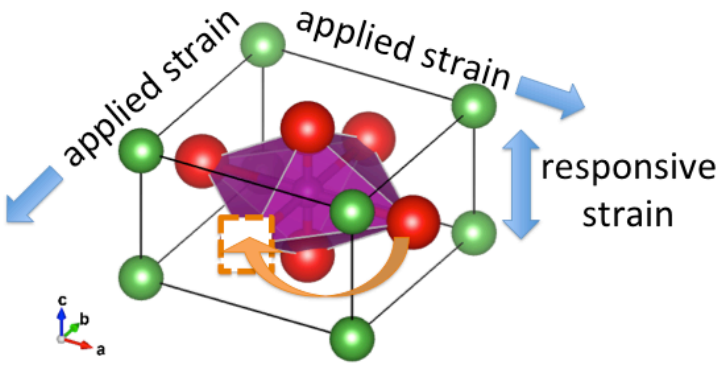
HTCondor High Throughput Computing

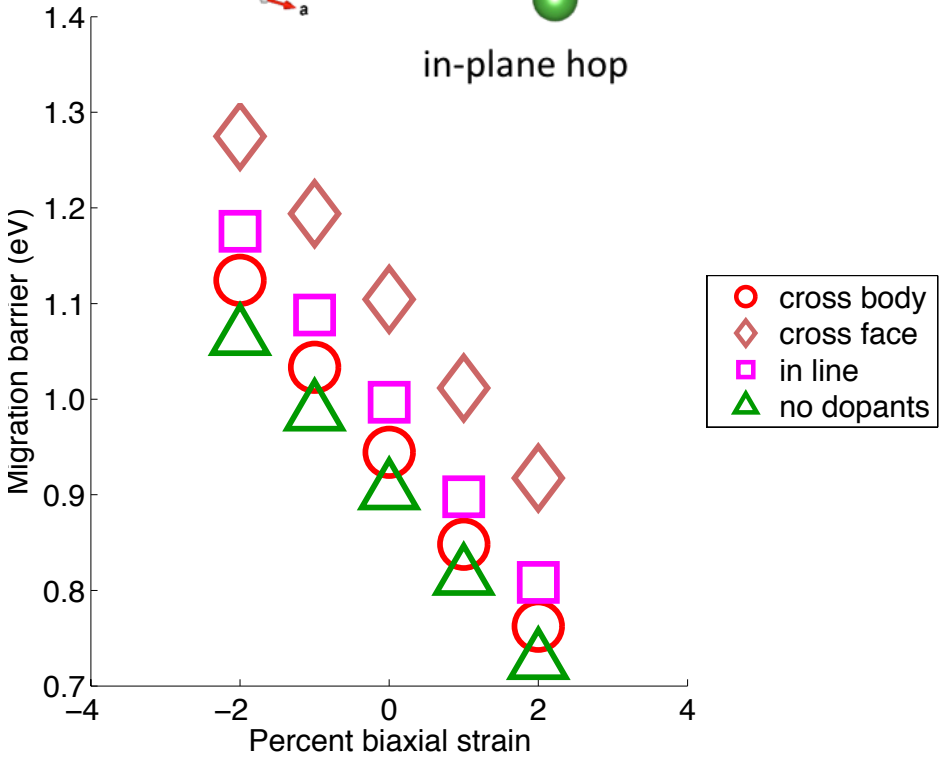
- Low headnode load
- Process-independent job monitor
  - Does not require a continuous process
  - Monitor gets information from text files: stable
  - Rebuilt each time: can be interrupted or fail without severe consequences
- Install and run without root access

Iterate easily over calculation system features



O_3





Same perovskite oxygen migration barrier workflow applied to different chemical systems, strain states, and dopant positions

Mayeshiba, T. & Morgan, D. *PCCP* **17**, 2715 (2015).

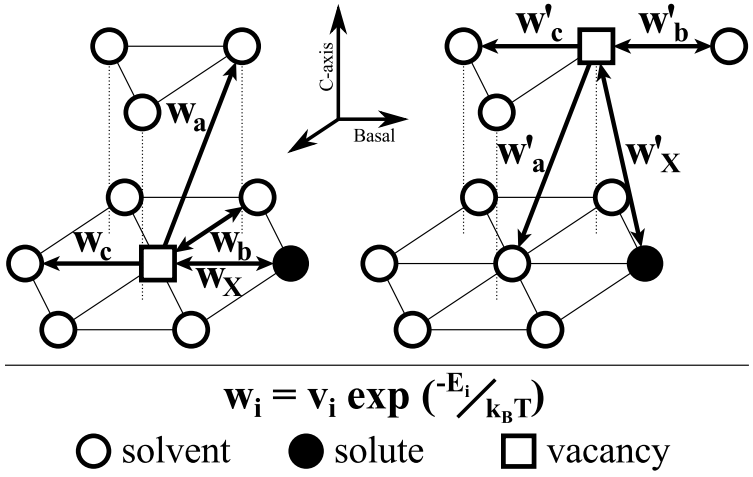
Store and share workflow knowledge

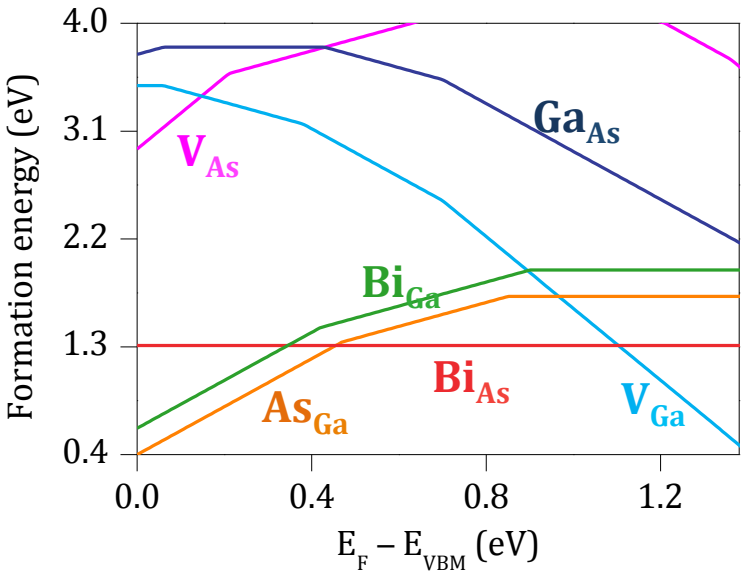
Extensive out-of-the-box functionality

- Full diffusion coefficient workflow
  - Phonons
  - Multiple hops
  - Frequency models for diffusion
- Full defect formation energy workflow
  - Charged defects
  - Finite size scaling
  - Potential alignment

Save custom workflows for future use

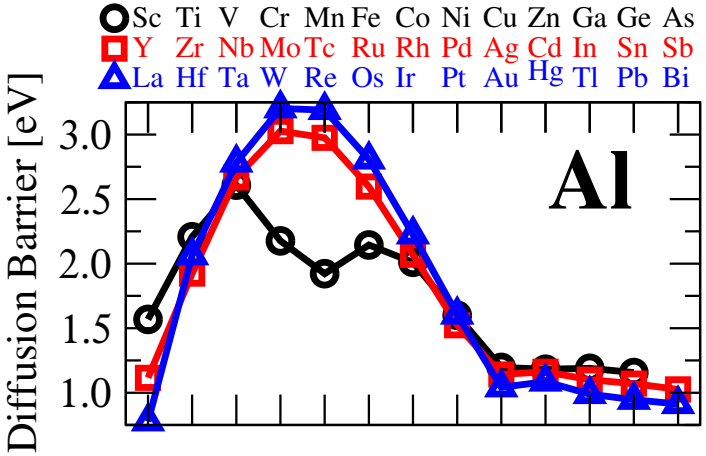
- Input file saved with data
- Reproduce results

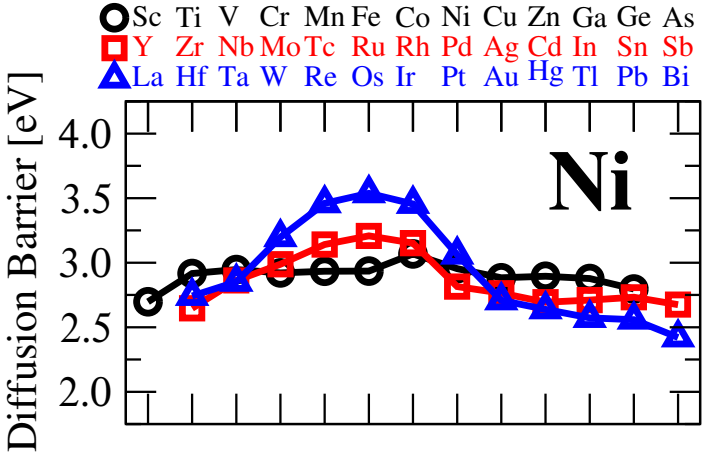




Produce highly-organized, consistently-calculated data

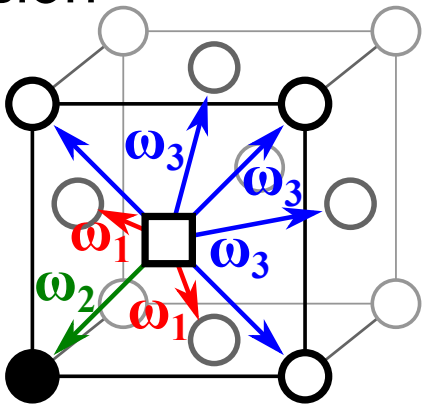
Example: Dilute solute diffusion

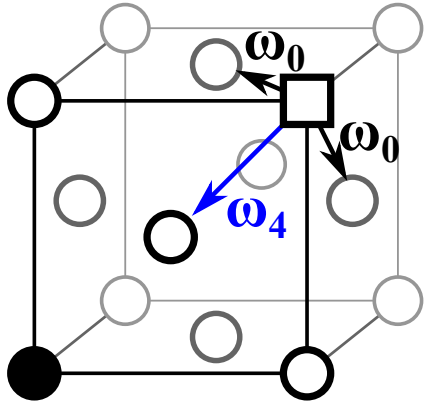


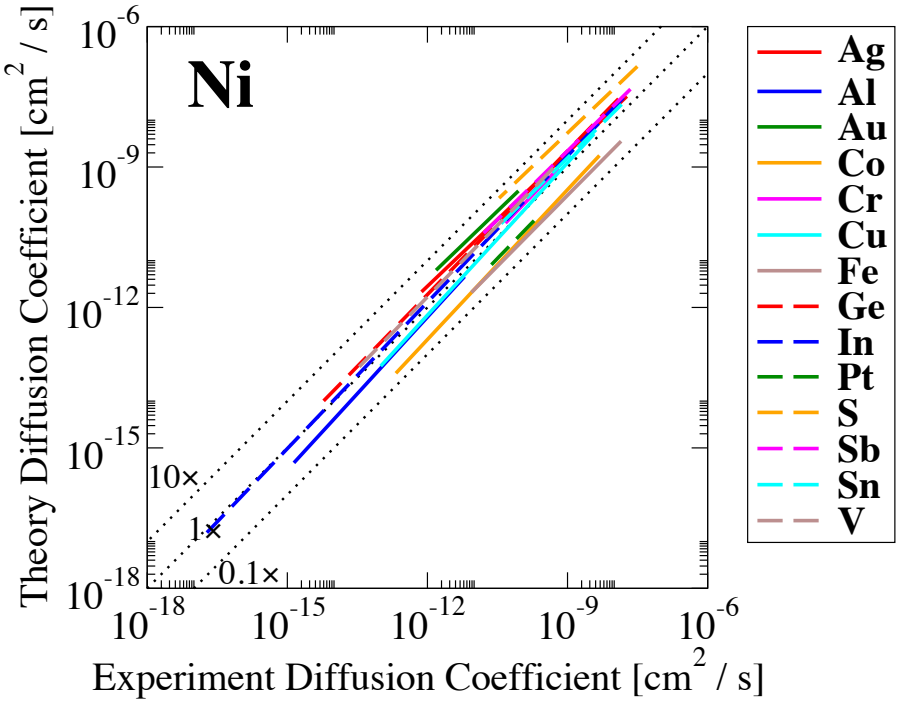


7 hosts (5 FCC, 1 HCP, 1 BCC)

> 230 host-solute combinations

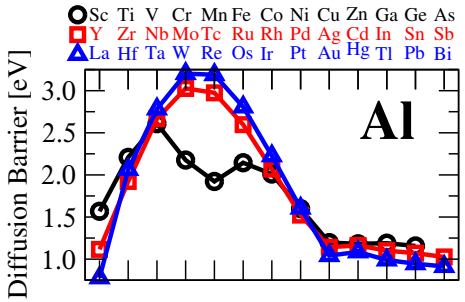




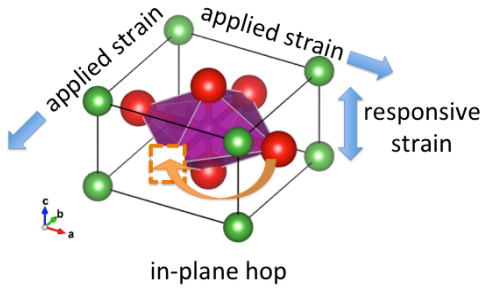


diffusiondata.materialshub.org; H. Wu et al., Scientific Data (2016, accepted).

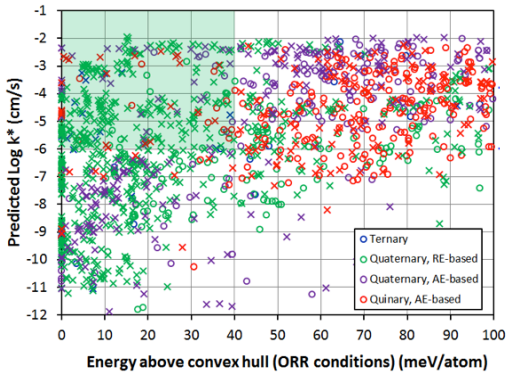
Scale examples of MAST-generated data



- Solute diffusion[1]: 20-30 steps per workflow x 230+ host-solute systems => over 6000 calculations



- Perovskite oxygen migration, with and without strain[2,3]: 15-25 steps per workflow x 200+ workflows and 392 steps per workflow x 4 systems => over 5000 calculations



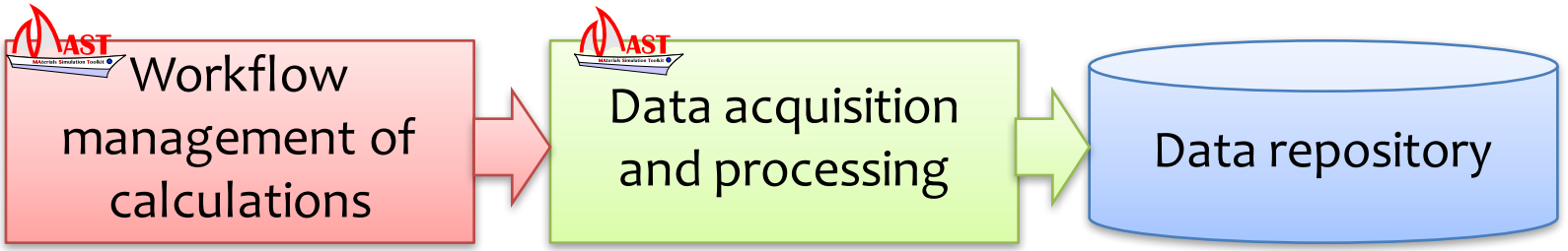
- Surface exchange coefficient descriptor in perovskites[4]: 3 steps per workflow x 1850+ compositions => over 5500 calculations

MAST is good for handling complex workflows and for copying workflows over many systems.

MAST MAterials Simulation Toolkit

[1] H. Wu et al., Scientific Data (2016, accepted)
[2] T. Mayeshiba & D. Morgan, *PCCP* **17**, 2715 (2015)
[3] T. Mayeshiba & D. Morgan, in preparation
[4] R. Jacobs et al., in preparation

Storing MAST-generated data



3-30 steps per workflow

200-1850 workflows per data set

5000-6000 calculations per data set, 5-30 GB

Archived data

- NIST Data repository
  - http://hdl.handle.net/11256/102
  - http://hdl.handle.net/11256/76
- Figshare
  - https://dx.doi.org/10.6084/m9.figshare.1546772.v2
- Zenodo
  - https://dx.doi.org/10.5281/zenodo.48656
- Materials Data Facility/Globus?

Interactive data

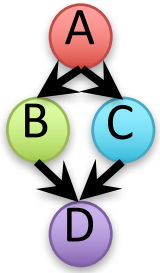
- Own dilute solute diffusion database website http://diffusiondata.materialshub.org
- Materials Project dataset: MPContribs (in progress)
- Citrine/Citrination?

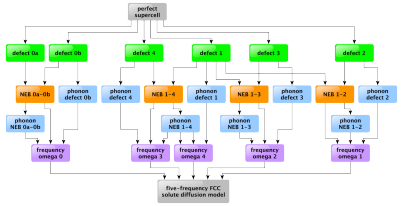
Consolidation strategies?

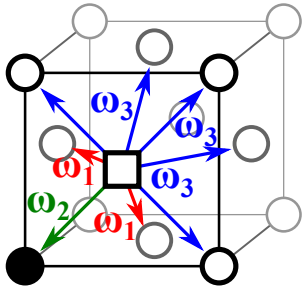
Summary

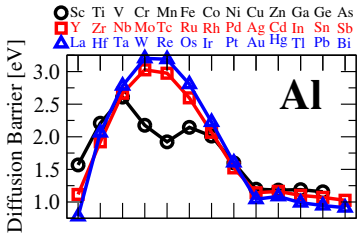
MAST was built to:

- Automatically manage workflows
- Iterate easily over calculation system features
  - Composition, strain, defects
- Store and share workflow knowledge
  - Included workflows emphasize diffusion and defect calculations
  - Almost all VASP calculations can be automated using MAST
- Produce highly organized, consistently calculated data









Github repository: http://github.com/uw-cmg/MAST
Documentation: http://www.pythonhosted.org/MAST
Python Package Index: http://pypi.python.org/pypi/MAST

MAST
MAterials Simulation Toolkit

Acknowledgements

COMPUTATIONAL MATERIALS GROUP

Faculty

* **Izabela Szlufarska**
* **Dane Morgan**

Postdocs

* Georgios Bokas
* Guangfu Luo
* Henry Wu
* Jia-Hong Ke
* Mahmood Mamivand
* Ryan Jacobs
* Shipeng Shu
* Wei Xie
* Yueh-Lin Lee

Graduate Students

* Amy Kaczmarowski
* Ao Li
* Austin Way
* Benjamin Afflerbach
* Chaiyapat Tangpatjaroen
* Cheng Liu
* Franklin Hobbs
* Hao Jiang
* Huibin Ke
* Hyunseok Ko
* Jie Feng
* Lei Zhao
* Mehrdad Arjmand
* Shenzhen Xu
* Shuxiang Zhou
* Tam Mayeshiba
* Xing Wang
* Yipeng Cao
* Zhewen Song

Visiting and Undergraduate Students

* Aren Lorenson
* Benjamin Anderson
* Haotian Wu
* Jason Maldonis
* Josh Perry
* Jui-Shen Chang
* Liam Witteman
* Tom Vandenberg
* Zachary Jensen

T. Mayeshiba: NSF GRFP DGE-0718123,
UW-Madison GERS
H. Wu, Z. Song, B. Afflerbach: NSF SI2-SSI 1148011
Calculations: UW-Madison Center for High Throughput Computing; University of Kentucky Lipscomb Center; NERSC DE-AC02-05CH11231