materials design®

High Value from High Throughput:

Harness the Power of LAMMPS with MedeA®

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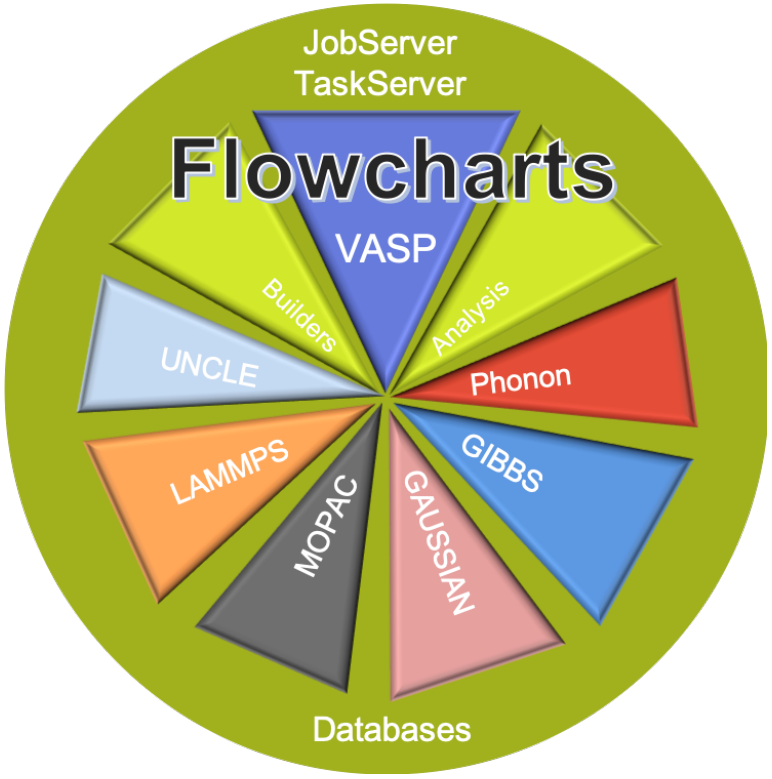
Materials Design

LAMMPS Workshop
15 August 2019

MedeA® Software Environment

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
- Force Fields (potentials)
  - 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

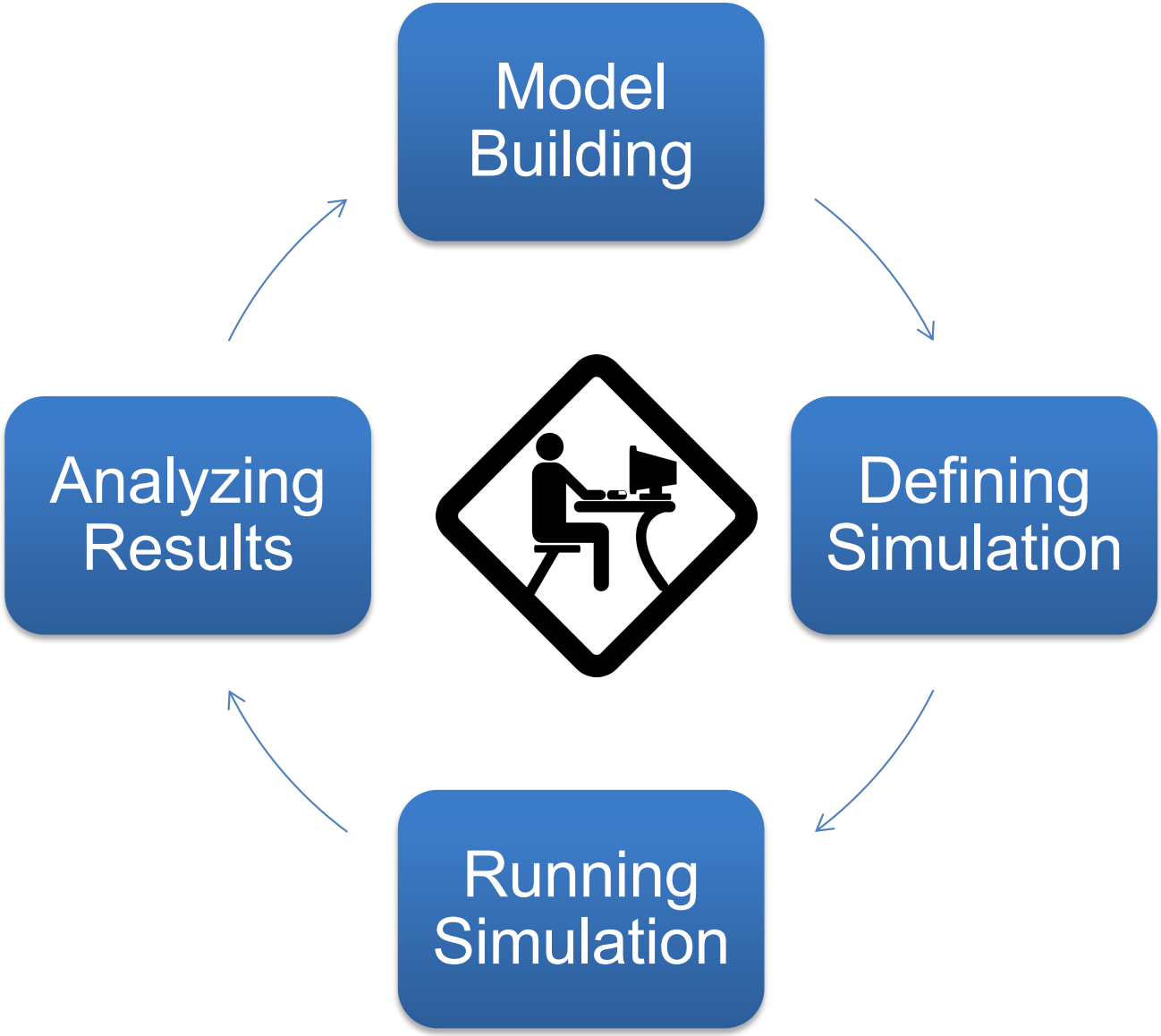


Potentials in MedeA

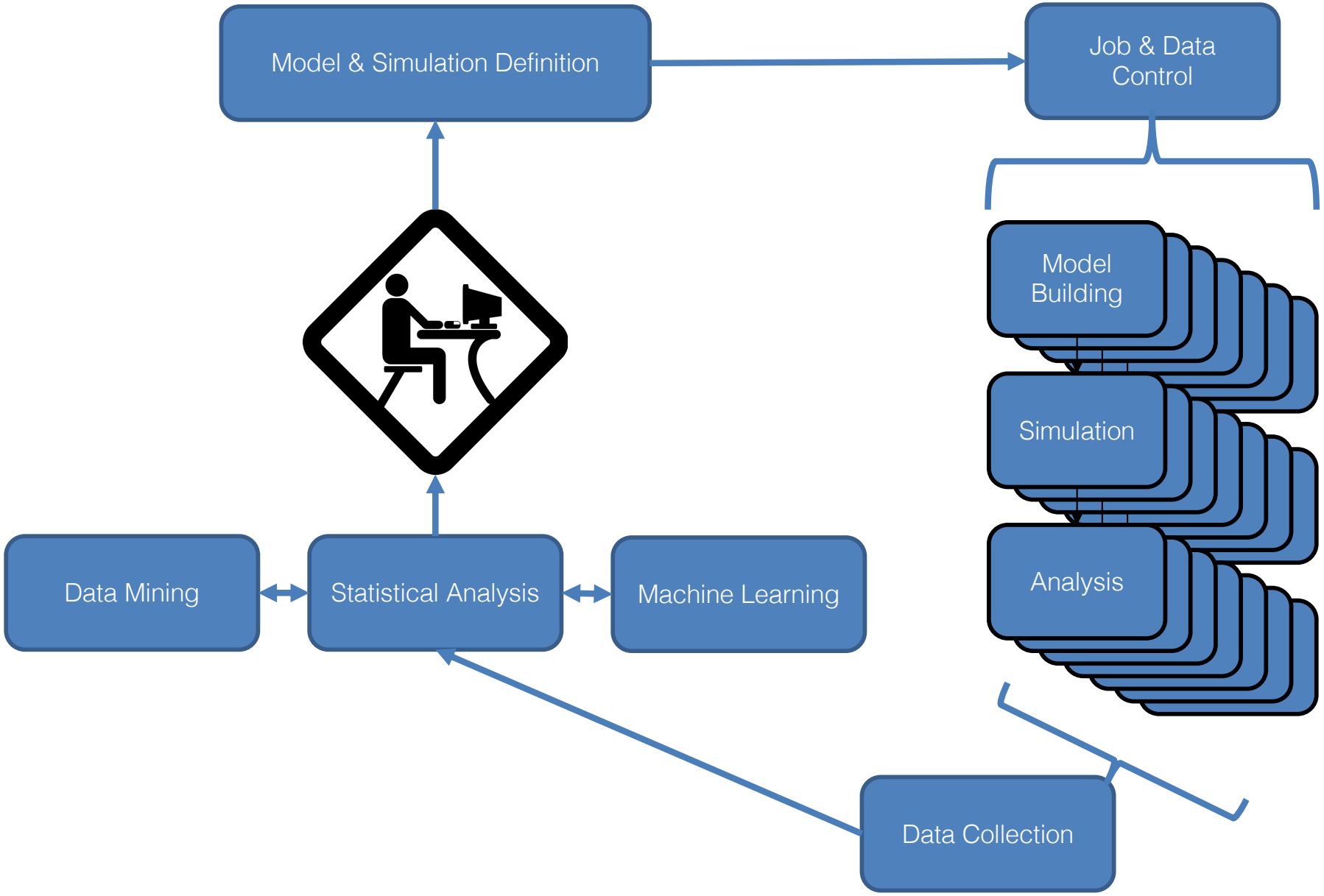
- Metallic forcefields:
  - EAM
    - All LAMMPS eam, eam/fs, and eam/alloy variants
  - MEAM
- Inorganic forcefields:
  - Buckingham
  - BKS
  - Clay-FF
  - CVFF_aug
- Semiconductor forcefields:
  - Tersoff
  - Stillinger-Weber
  - REBO
- Organic (valence) forcefields:
  - PCFF/PCFF+*
  - Compass/Compass+
  - OPLS-AA/OPLS-AA+*
  - AUA/AUA+ *
  - Trappe+ *
- Variable charge forcefields
  - Streitz-Mintmire
  - COMB3
  - ReaxFF
- All other potentials in LAMMPS can be invoked via some additional lines of LAMMPS commands

* **Also available in MedeA®-GIBBS**

Current Approach…



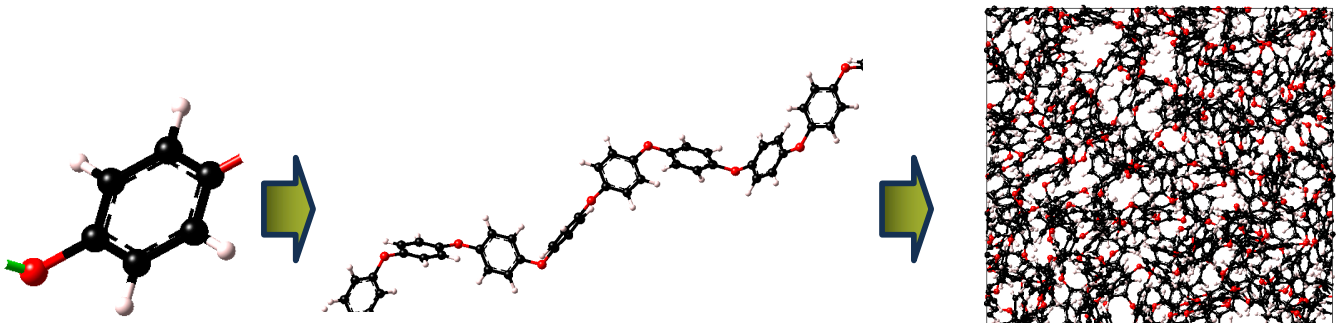
… Going to High-Throughput



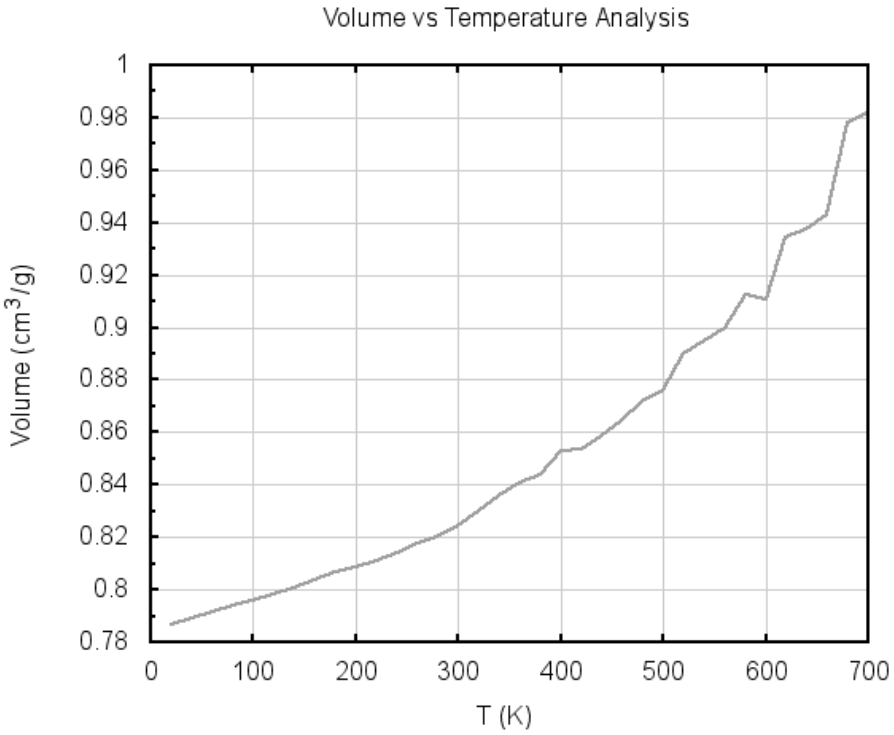
Warmup:

T_g of PPE

Glass Transition T_g of a Polymer

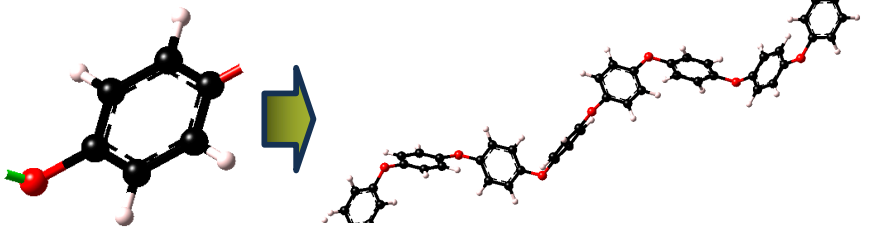


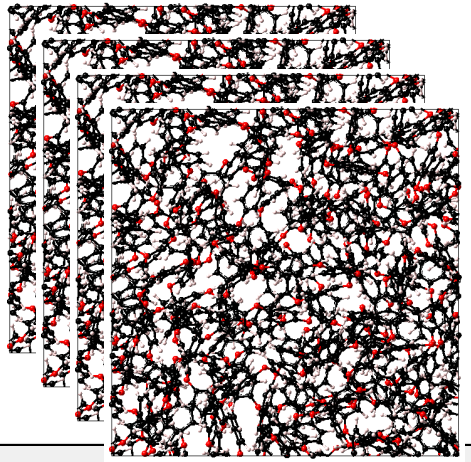
Polyphenylene ether (PPE)



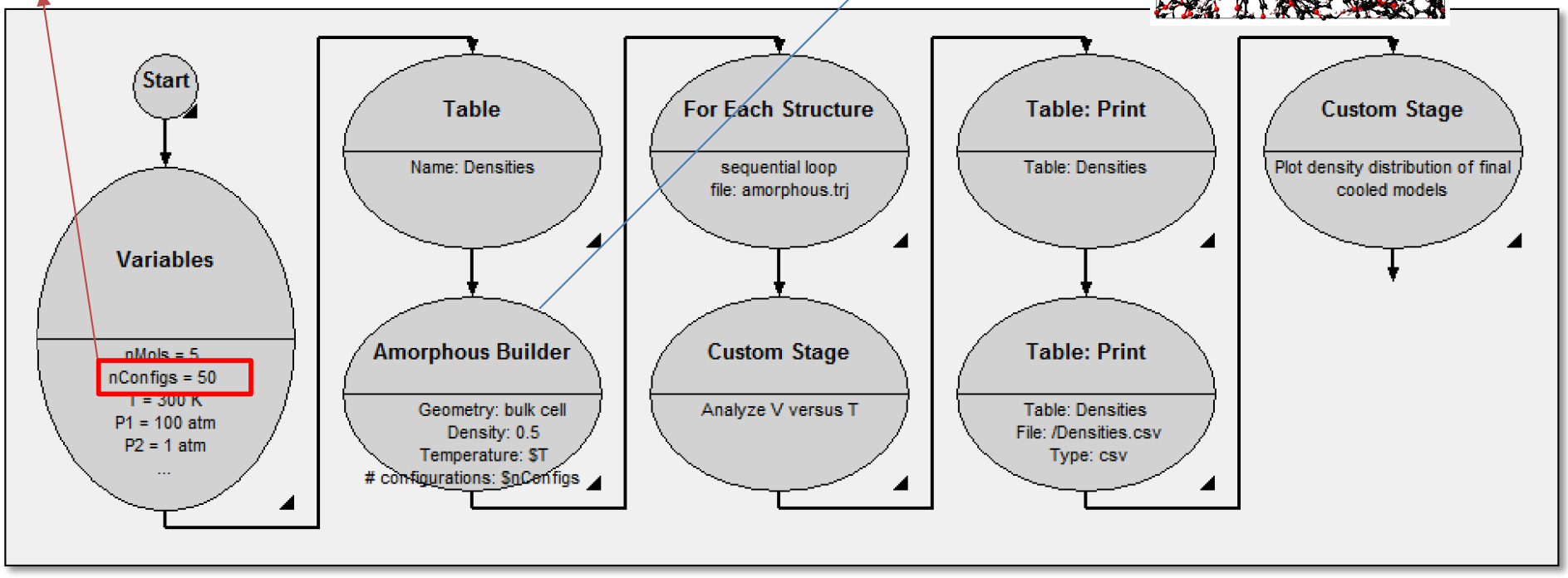
Where is the T_g?

Amorphous System V vs T

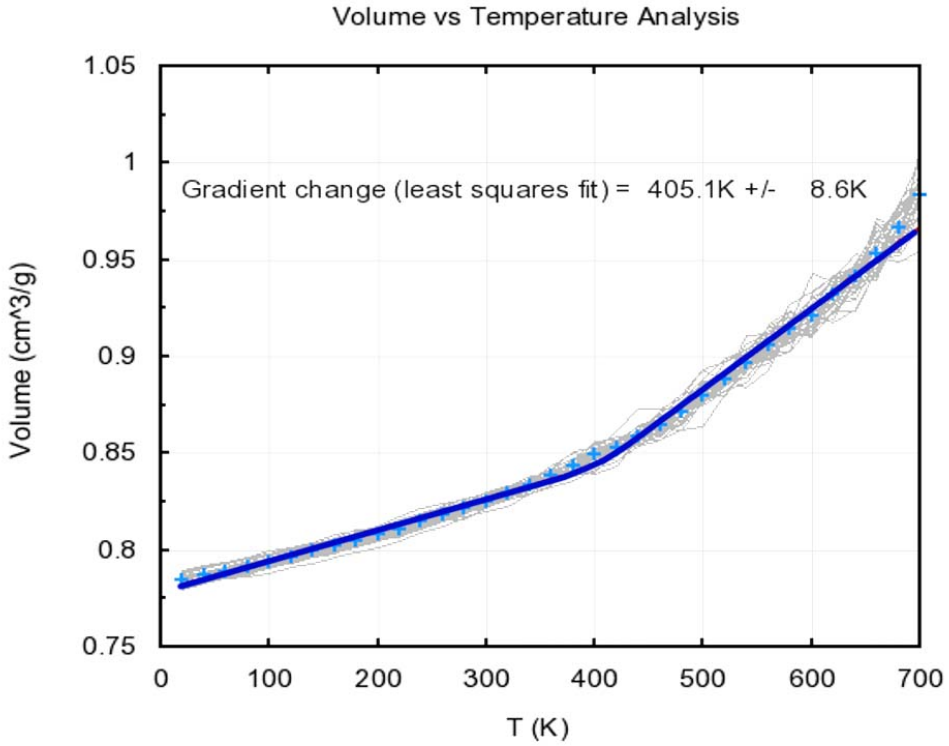




Automatically build 50 configurations



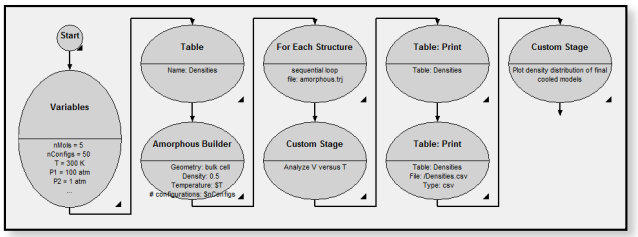
Glass Transition T_g of a Polymer



Value of high throughput calculations:

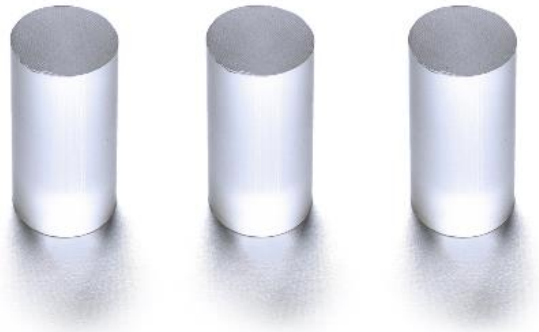
- Clear signal from noisy simulation data

- Variability in individual V vs. T curves (gray lines)
- Fit yields properties for the simulated system
- Automatic procedure: single high throughput flowchart



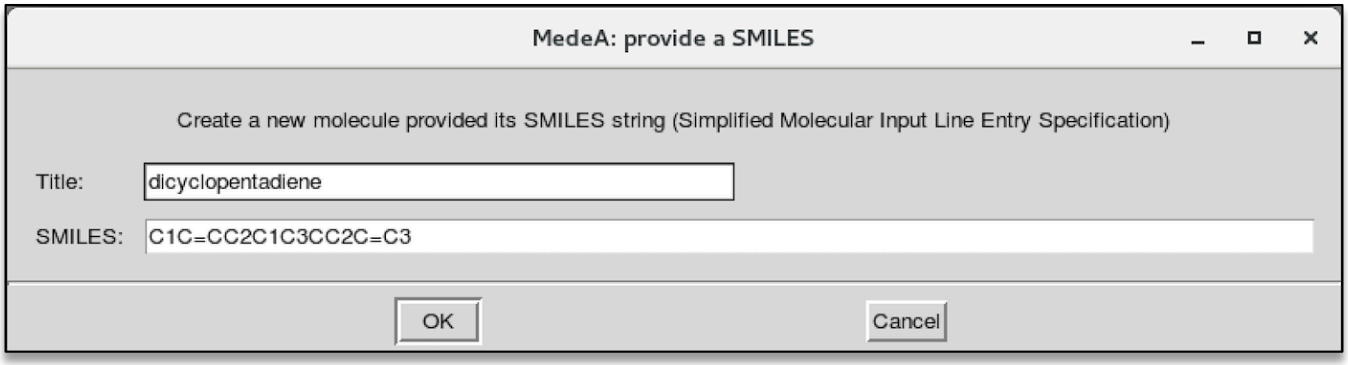
High-throughput Sampling:

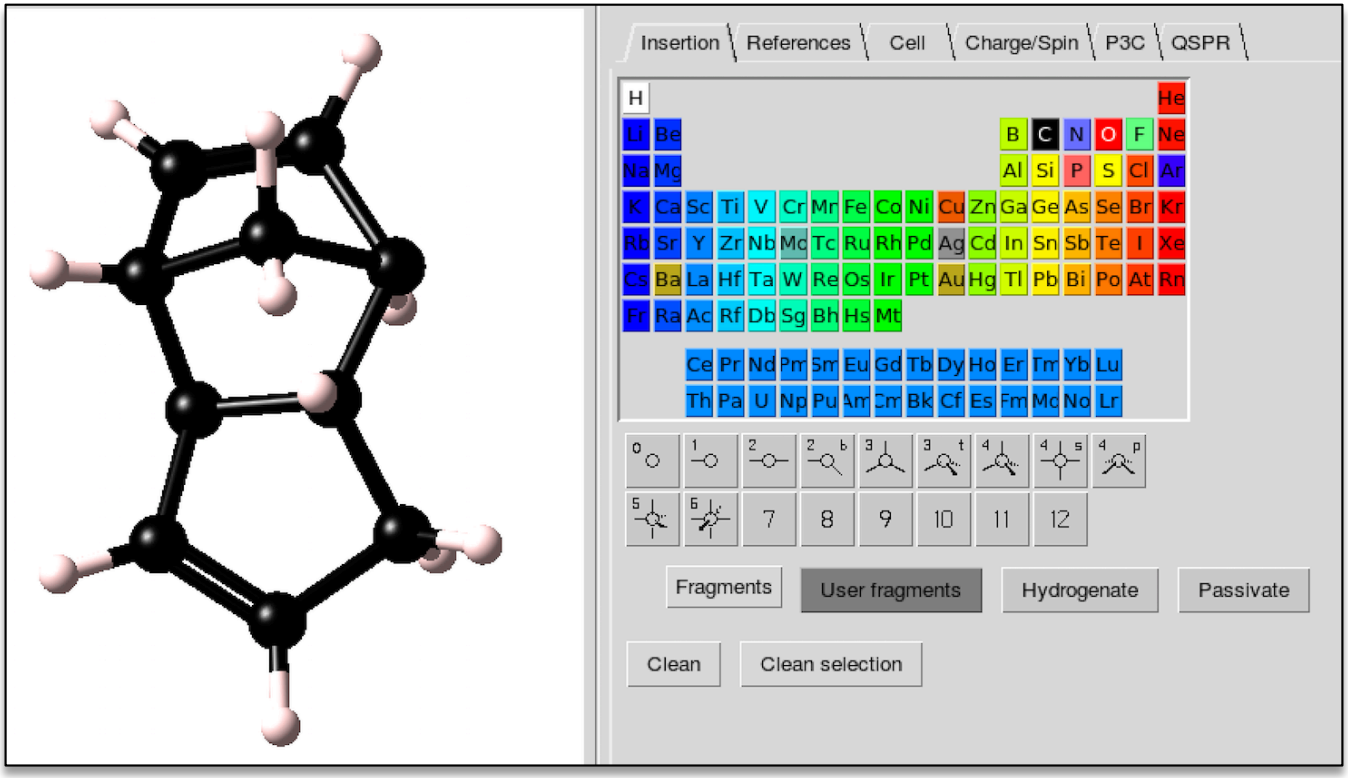
Mechanical properties of a high performance thermoset resin



Building a Monomer

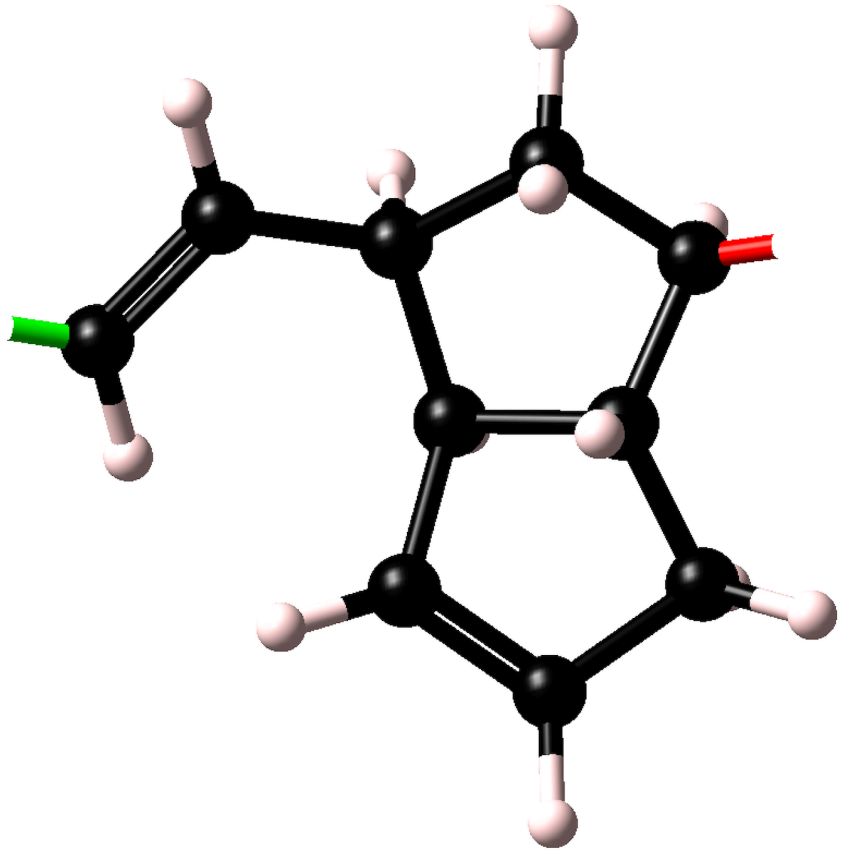
- Use the SMILES string





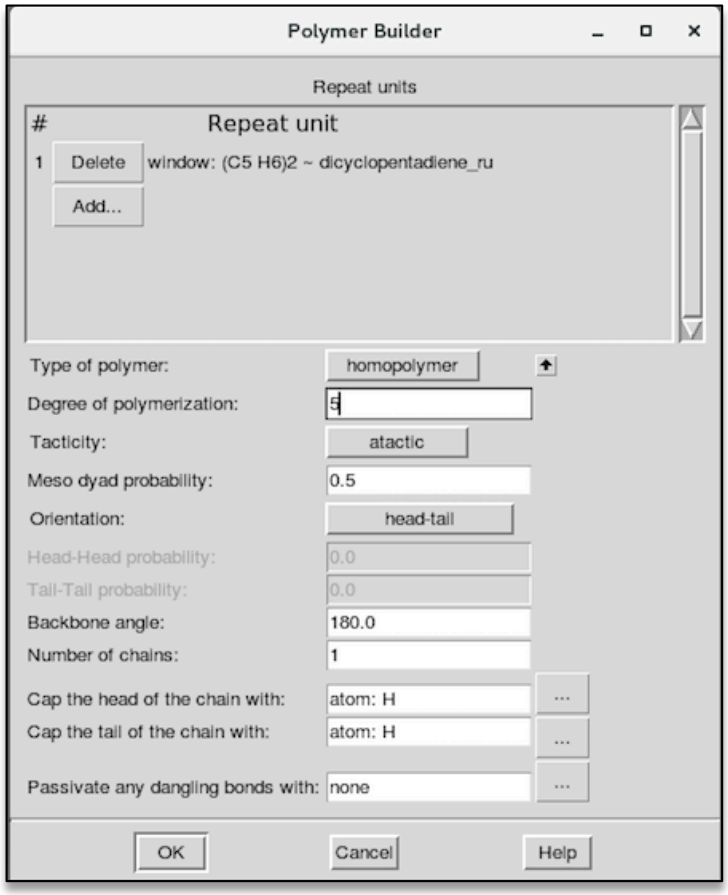
Modifying into a Repeat Unit

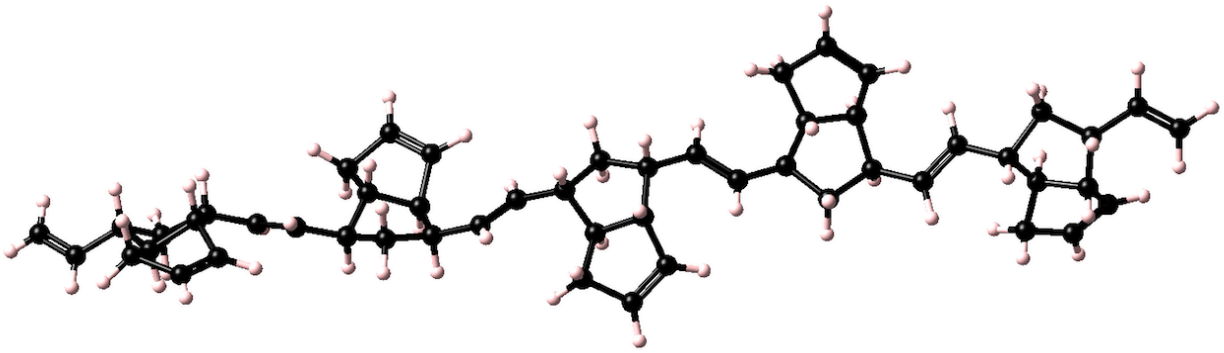
- Edit into a repeat unit with the Molecular Builder
  - Break bond, delete H atoms, then define a repeat unit



Turning into a Polymer

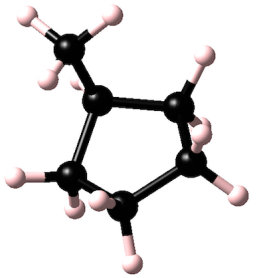
- Build with MedeA Polymer Builder
  - DP = 5 in this example

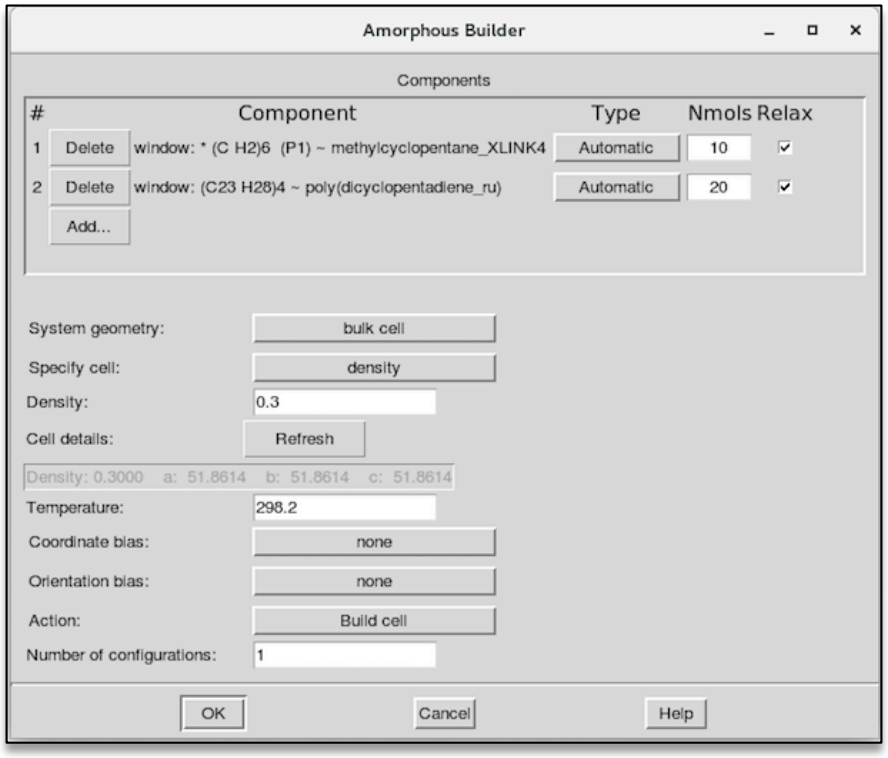


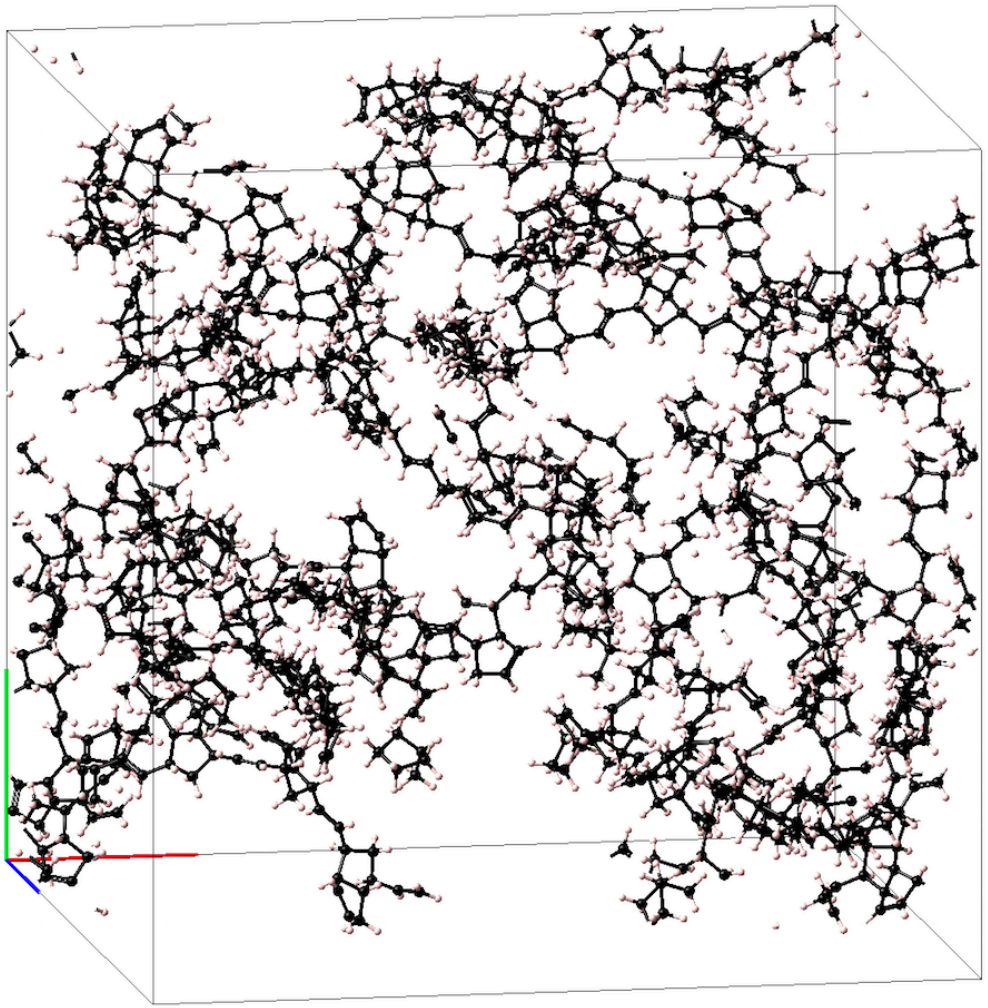


Building Initial Amorphous Material

- Use MedeA Amorphous Materials Builder
  - Combine poly(dicyclopentadiene) with cross-linkers



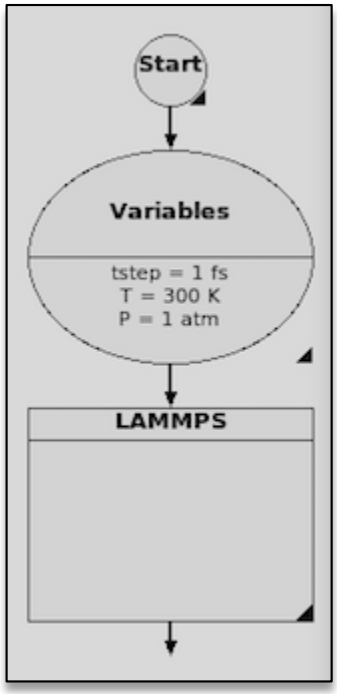


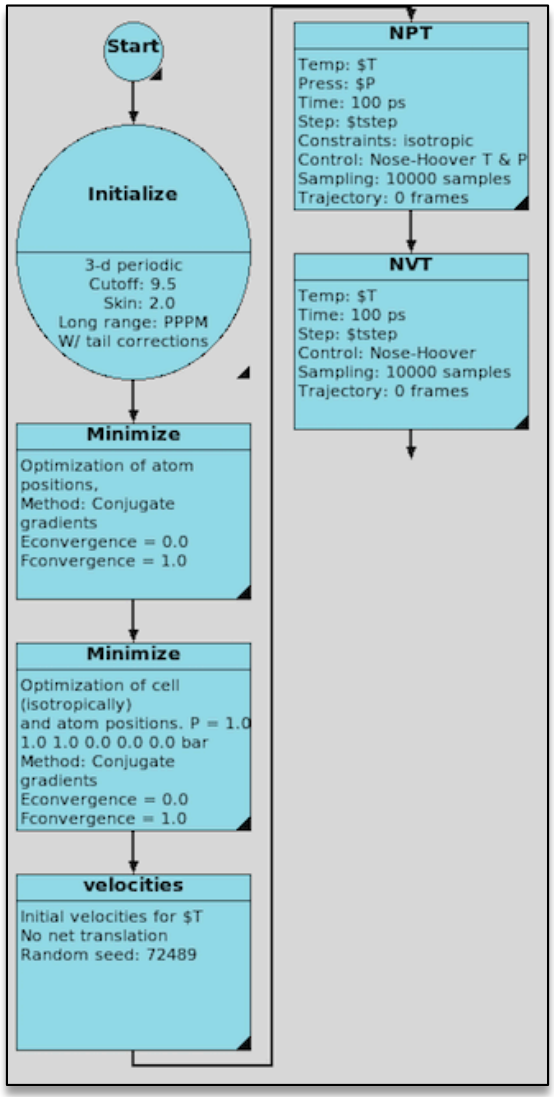


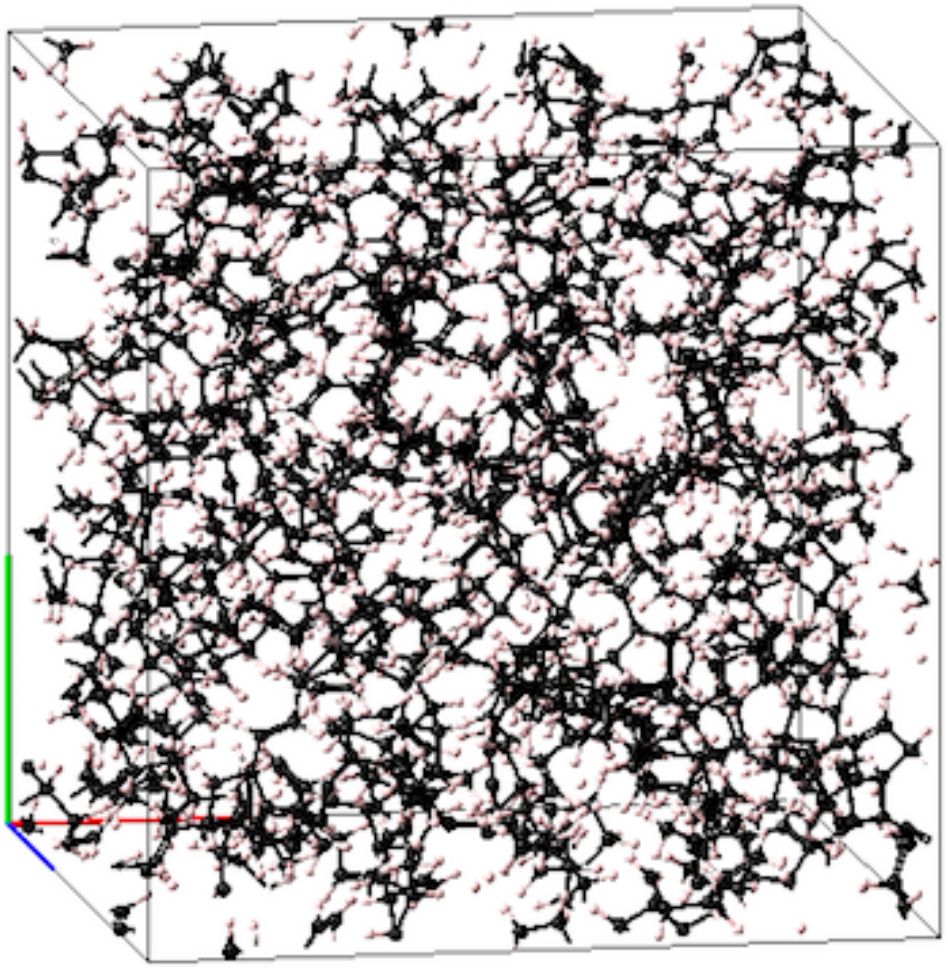
Initial density: 0.3 g/cc

Equilibrating the Amorphous Material

- With MedeA LAMMPS using PCFF+ forcefield
  - Design simulation workflow with Flowchart



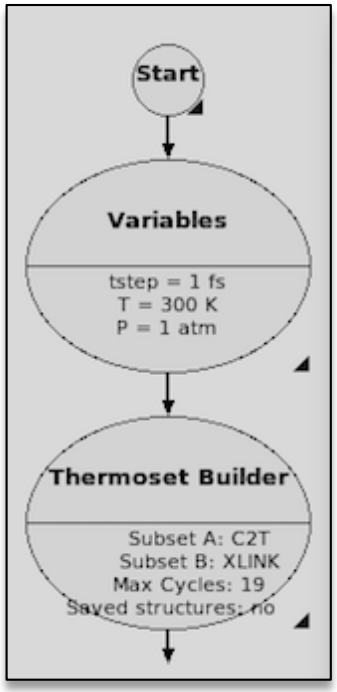


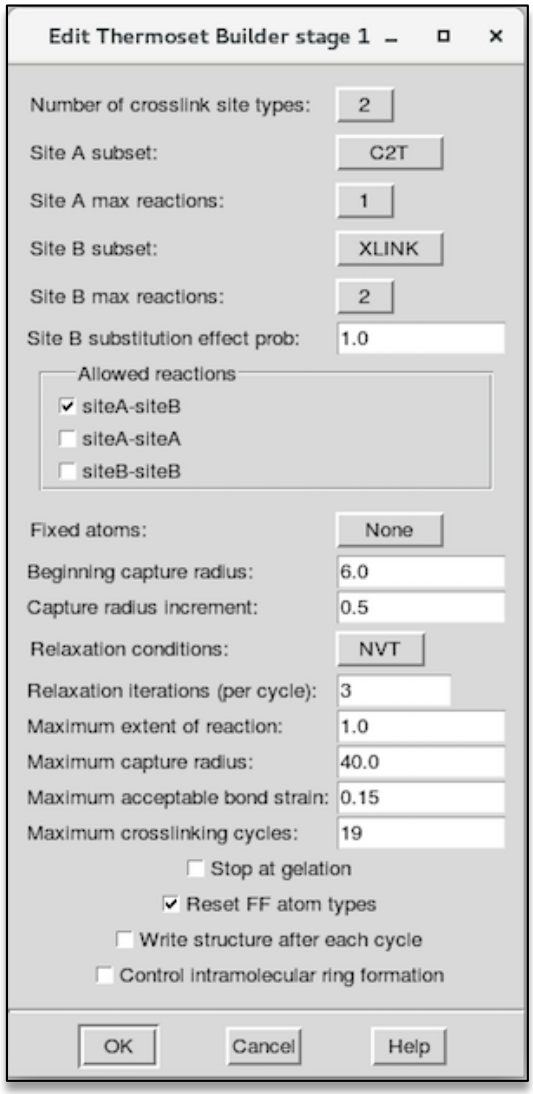


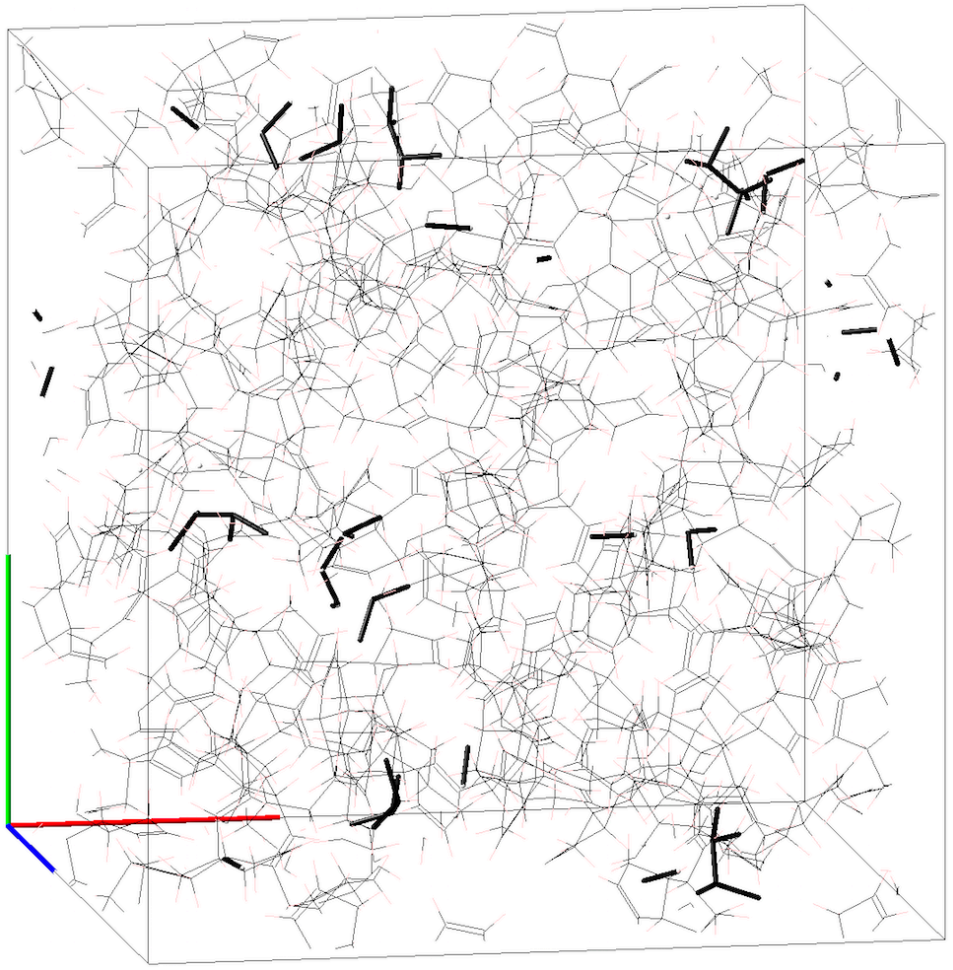
Equilibrium density at 300K: 0.963 g/cc

Creating Cross-links

- With MedeA Thermoset Builder

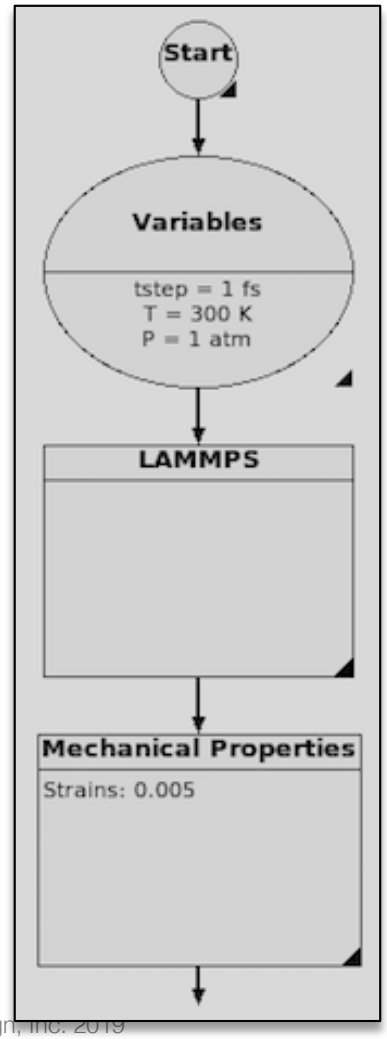


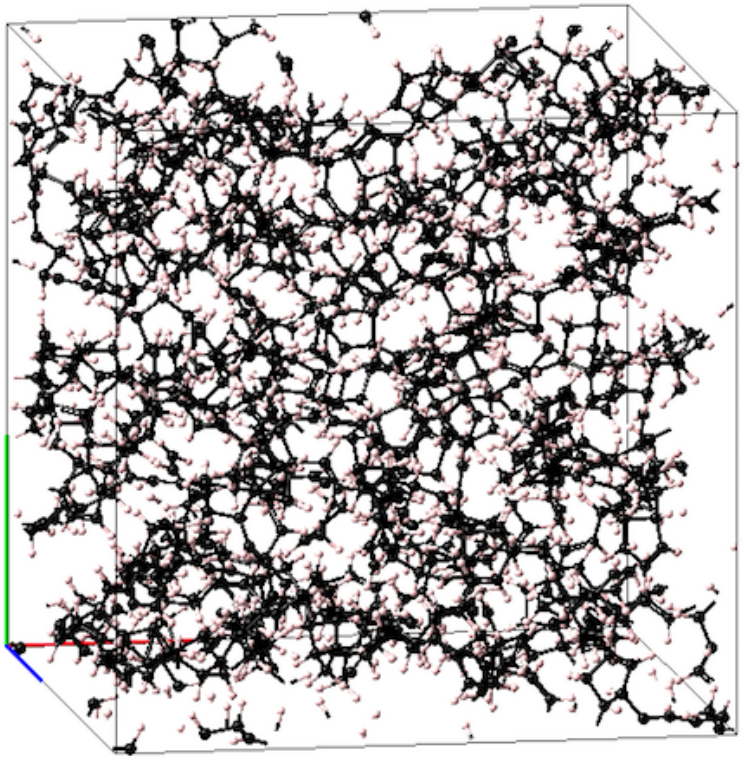




Predicting Mechanical Properties

- Final equilibration and calculate mechanical properties
  - Includes elastic constants, modulus, and thermodynamic functions

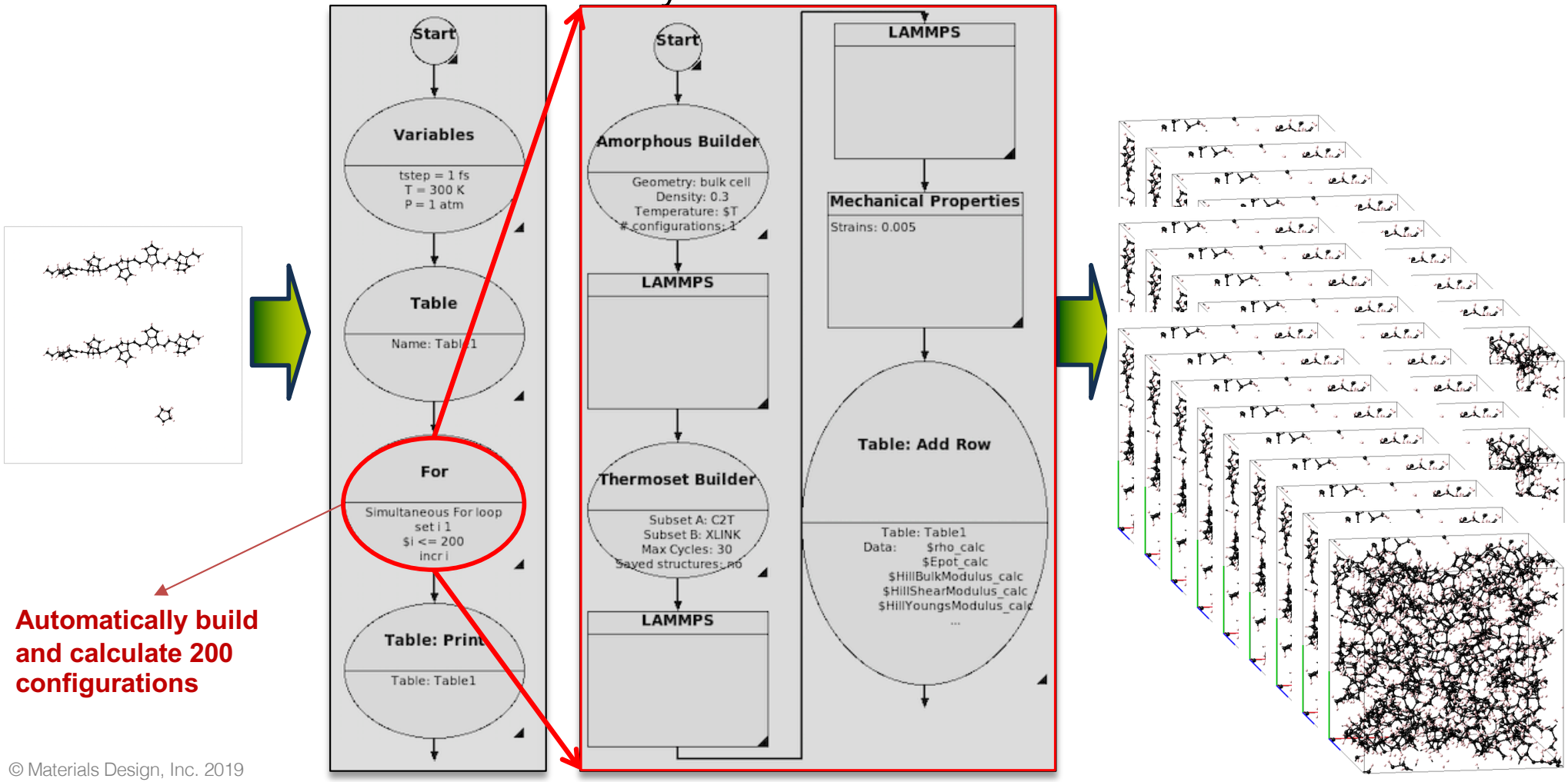




Modulus	Voigt	Reuss	Hill	
Bulk	2.13	1.99	2.06	GPa
Shear	1.20	1.02	1.11	GPa
Young's	3.03	2.61	2.82	GPa
Longitudinal	3.73	3.35	3.54	GPa

High-Throughput Sampling

- Use MedeA High-Throughput Flowchart to turn 1 initial configuration to hundreds of samples and perform property calculations automatically



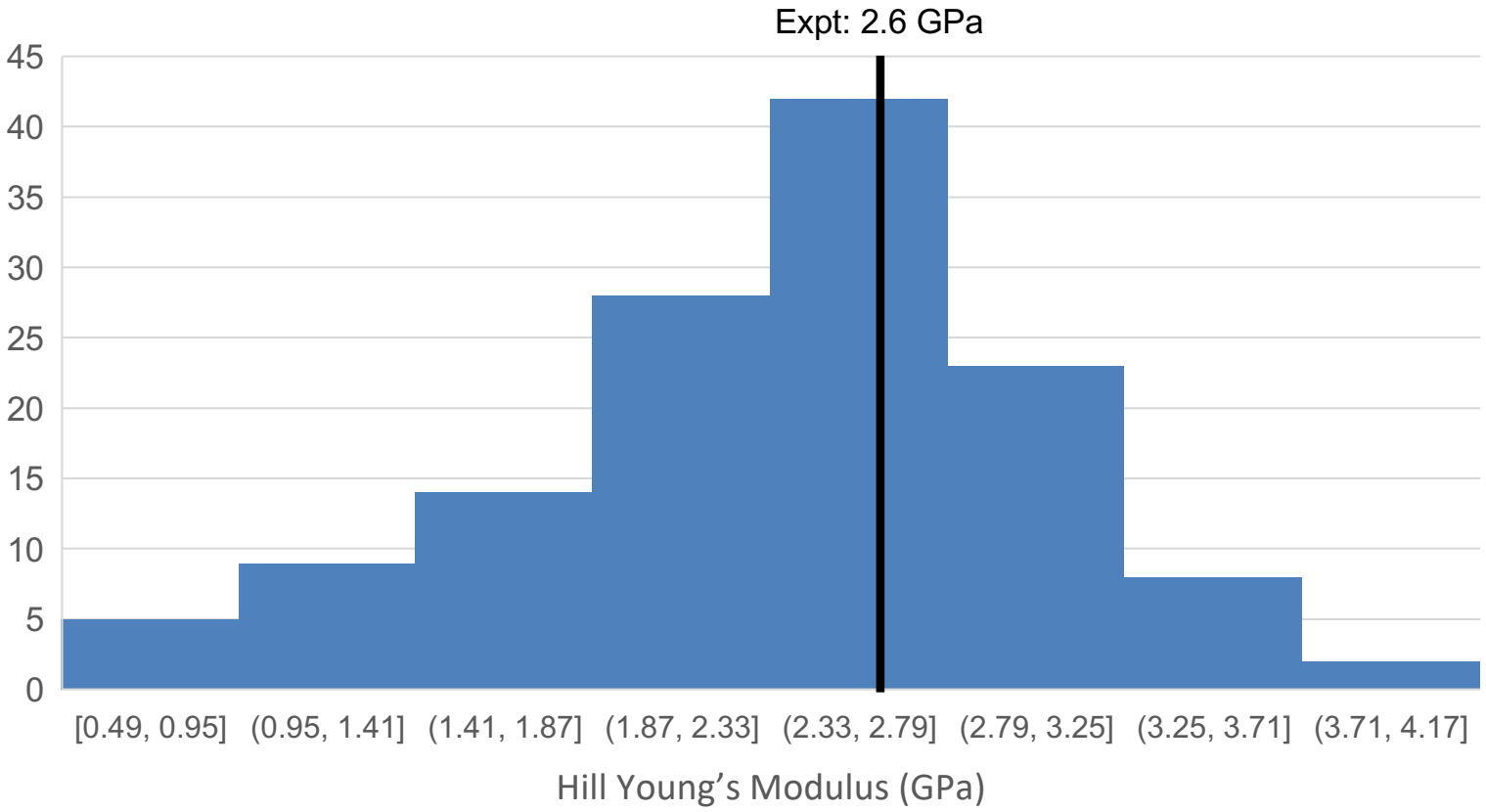
High-Throughput Sampling

- Results written in a table

Density g/cm^3	Energy kcal/mol	Hill Bulk Modulus GPa	Hill Shear Modulus GPa	Hill Young's Modulus GPa	Stability
0.913854	188.919249	2.51	1.63	4.02	1
0.911153	188.698989	0.52	0.50	1.23	0
0.977401	3809.325976	2.23	1.05	2.71	1
0.915711	191.200429	1.78	0.88	2.26	1
0.971271	3762.628469	2.76	1.41	3.62	1
0.971267	187.605648	2.49	1.86	4.47	1
0.979720	3515.846232	2.86	1.40	3.61	1
0.950648	3793.735874	2.62	1.24	3.21	1
0.907735	189.696099	2.60	1.46	3.68	1
0.905413	189.871619	-0.03	0.26	0.63	0
0.968701	3814.131277	2.49	1.41	3.55	1
0.968728	3817.210077	2.77	1.43	3.66	1
0.867437	194.550819	2.08	1.45	3.53	1
0.894680	192.374389	1.72	0.73	1.89	1
0.917270	188.726099	2.07	1.02	2.61	1
0.904528	190.810389	2.10	1.53	3.68	1
0.972136	3729.916964	2.79	1.46	3.73	1
0.958045	3768.324270	2.57	1.24	3.21	1
0.812593	189.164879	0.90	0.66	1.60	0
0.988430	3409.544716	2.71	1.37	3.51	1
0.964406	3754.486168	2.63	1.34	3.44	1
0.942615	188.046028	2.58	1.66	3.94	0
0.936354	188.777859	2.69	0.90	2.43	0
0.929796	187.961358	3.34	2.48	5.96	1
0.905169	189.972279	0.86	0.47	1.18	0
0.994661	190.813619	2.05	1.06	2.71	1
0.957068	3800.599375	1.80	1.05	2.63	1
0.973829	3854.690683	2.98	1.49	3.83	1
0.853735	194.565579	0.49	0.64	1.30	1
0.924945	193.050349	0.90	0.53	1.39	0
0.907131	191.455639	2.71	1.58	3.96	1
0.968984	3837.896280	3.07	1.55	3.99	1
0.851309	197.483850	0.75	0.34	0.82	0
0.932742	194.088279	8.12	3.00	7.89	0
0.948090	188.577459	2.19	1.07	2.61	0
0.862262	194.912639	0.42	0.13	0.39	0
0.971970	3854.994083	2.70	1.20	3.13	1
0.982627	3728.734764	2.68	1.04	2.75	1
0.903234	196.945560	2.64	1.12	2.88	0
0.959122	3849.152382	2.09	1.09	2.79	1
1.023171	185.480268	3.99	2.00	5.09	1
0.904138	189.875109	2.24	1.89	4.42	1
0.965173	3804.817875	2.60	1.42	3.61	1
0.960062	3849.761882	2.32	1.23	3.13	1
0.953017	3804.271575	2.41	1.26	3.22	1
0.889294	193.013059	2.11	-1.32	-14.32	0
⋮	⋮	⋮	⋮	⋮	⋮

High-Throughput Sampling

- Sampling over 200 configurations
  - 65.5% of the 200 samples were mechanically stable
  - Y in good agreement with experimental results of ~2.6 GPa

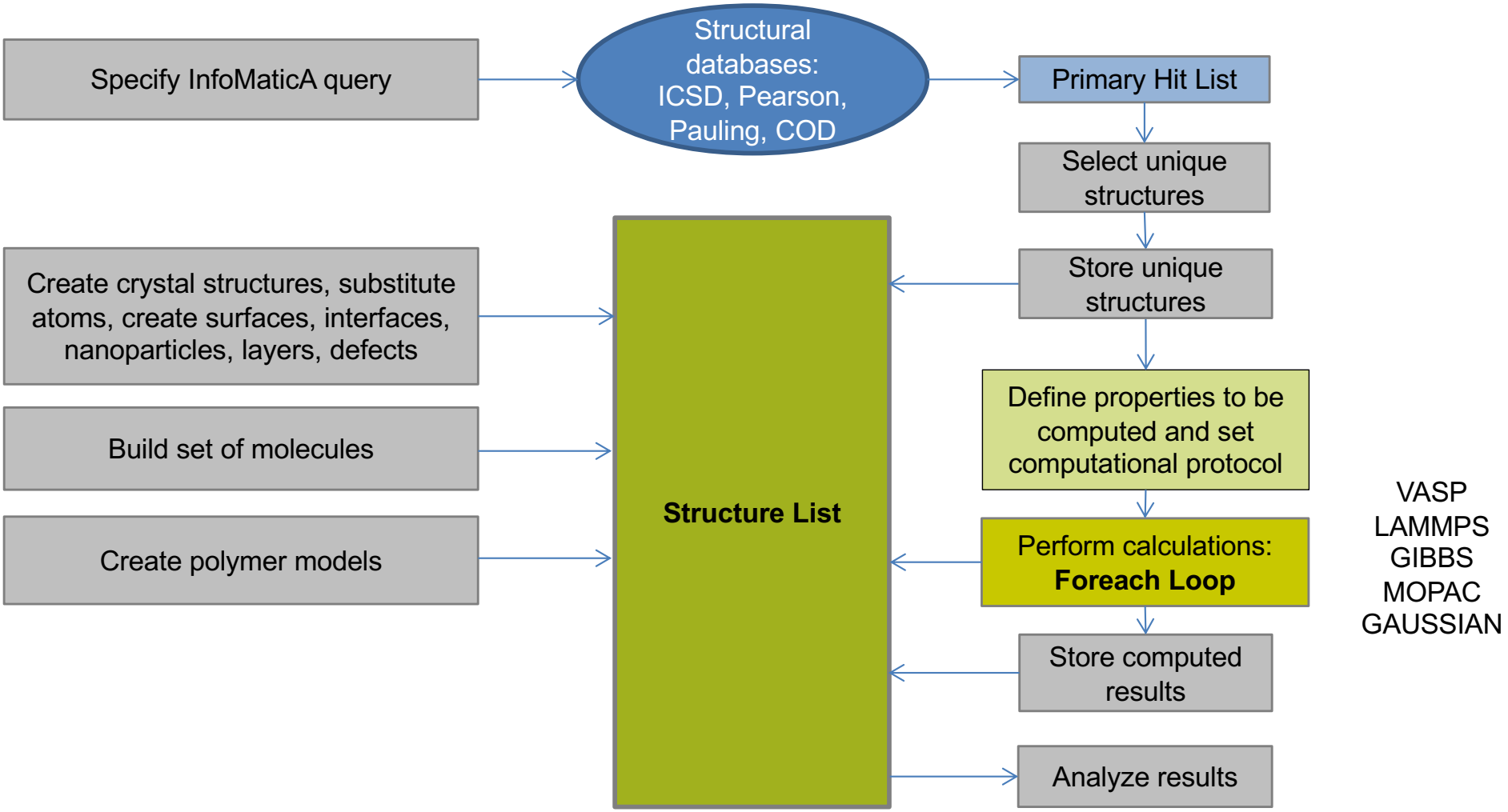


Summary

- Sampled through 200 cross-linked thermoset resins for their mechanical stability and elastic moduli
  - Generated 200 resin samples from 1 set of molecules and cross-linker
    - From molecules to amorphous materials to thermoset
  - Distribution of Young's modulus in excellent agreement with experiment

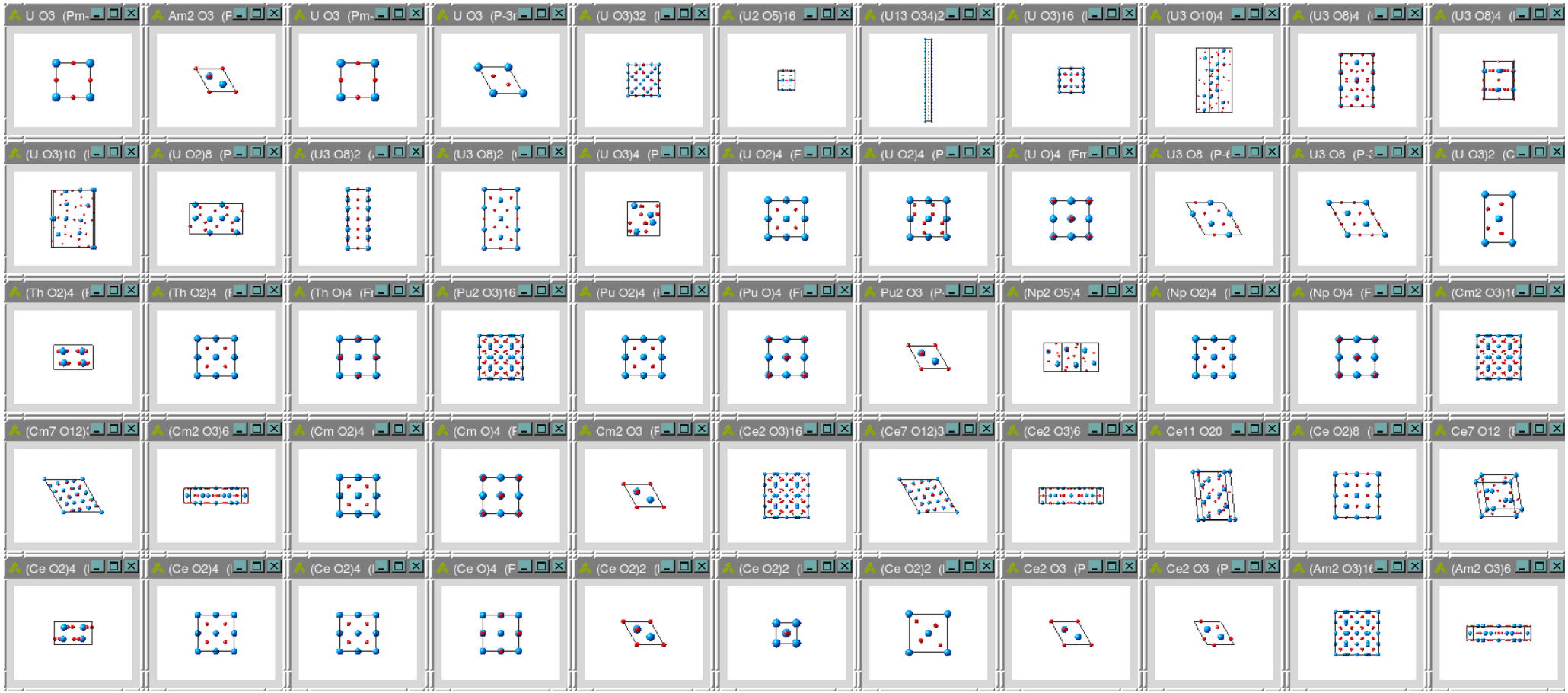
High-Throughput Screening

HT Implementation in MedeA



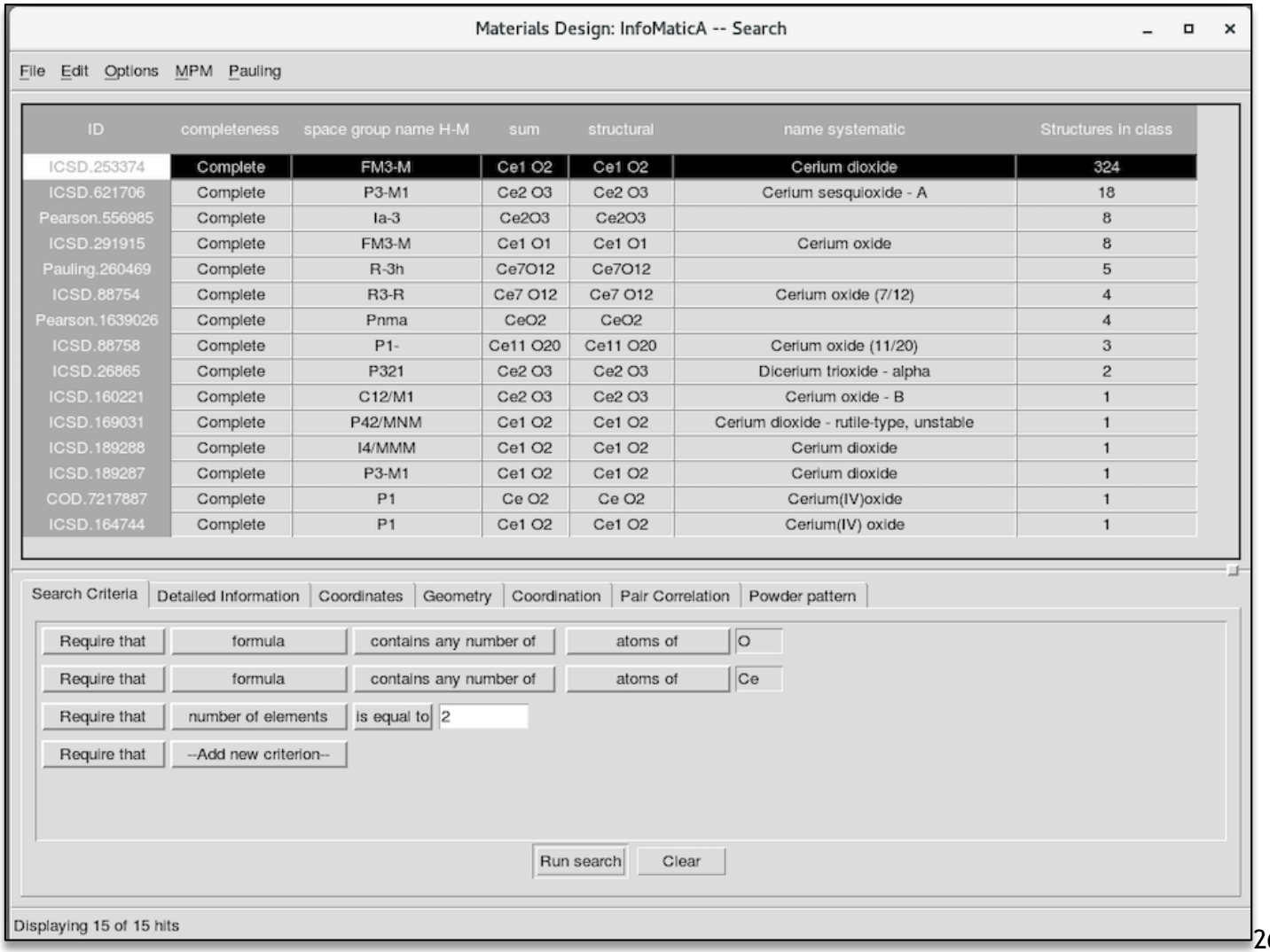
O Removal Energy of Actinide Oxides

- Ce/O, Am/O, Cm/O, Np/O, Pu/O, Th/O, and U/O compounds



O Removal Energy of Actinide Oxides

- Retrieve all Ce/O compounds
  - With MedeA® InfoMaticA



O Removal Energy of Actinide Oxides

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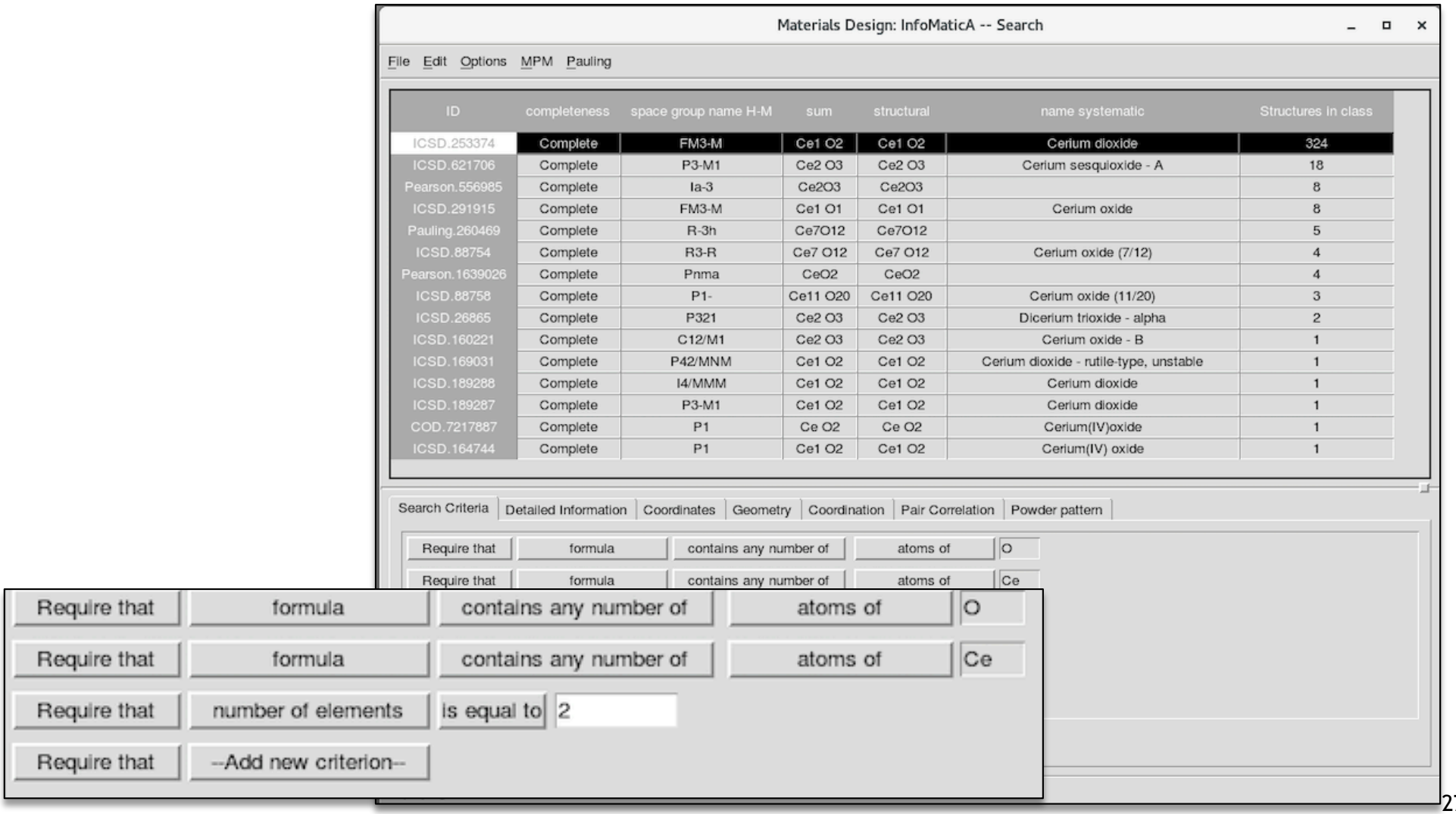
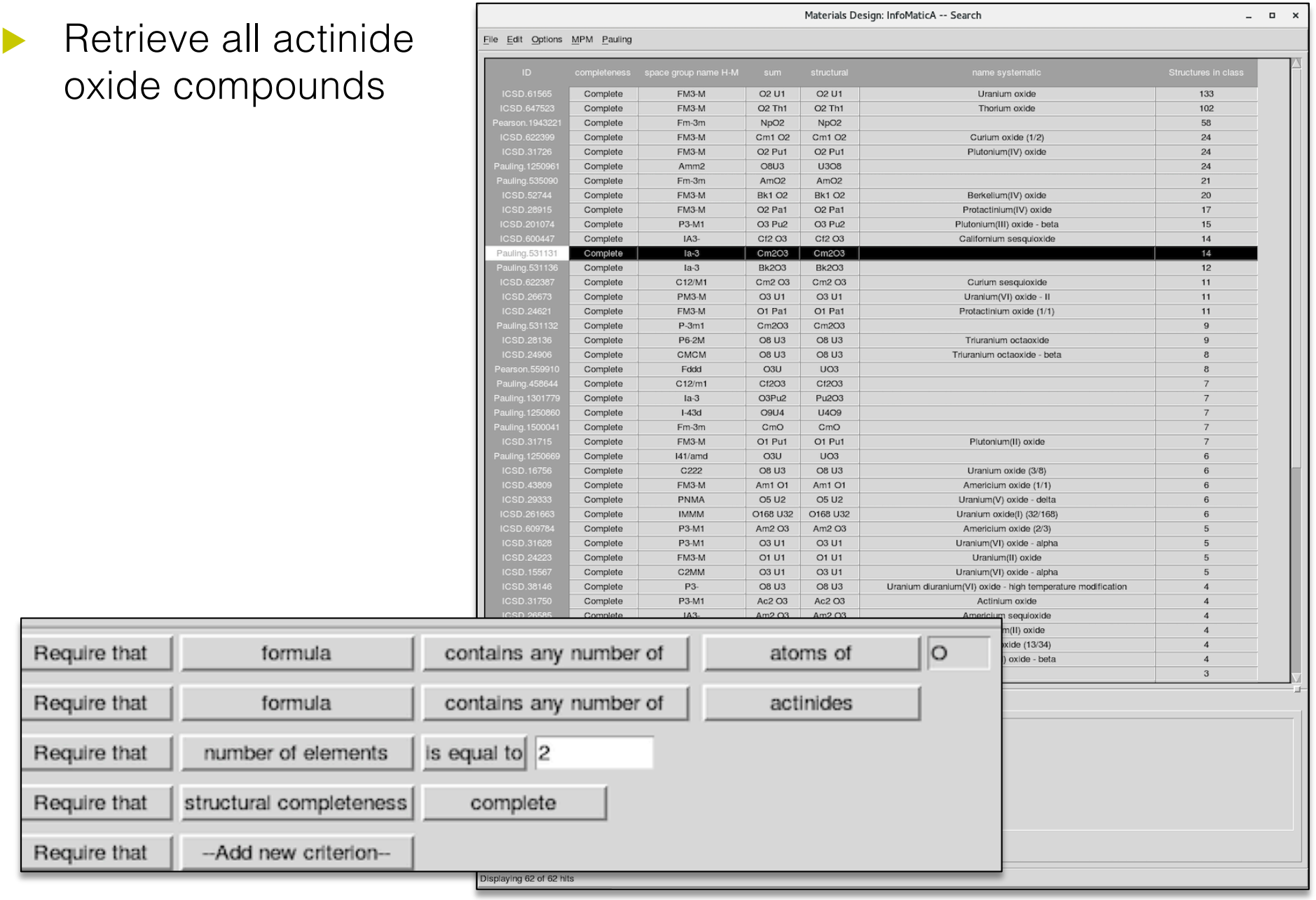


O Removal Energy of Actinide Oxides

- Retrieve all actinide oxide compounds



ID	completeness	space group name H-M	sum	structural	name systematic	Structures in class
ICSD.61565	Complete	FM3-M	O2 U1	O2 U1	Uranium oxide	133
ICSD.647523	Complete	FM3-M	O2 Th1	O2 Th1	Thorium oxide	102
Pearson.1943221	Complete	Fm-3m	NpO2	NpO2		58
ICSD.622399	Complete	FM3-M	Cm1 O2	Cm1 O2	Curium oxide (1/2)	24
ICSD.31726	Complete	FM3-M	O2 Pu1	O2 Pu1	Plutonium(IV) oxide	24
Pauling.1250961	Complete	Amm2	O8U3	U3O8		24
Pauling.535090	Complete	Fm-3m	AmO2	AmO2		21
ICSD.52744	Complete	FM3-M	Bk1 O2	Bk1 O2	Berkelium(IV) oxide	20
ICSD.28915	Complete	FM3-M	O2 Pa1	O2 Pa1	Protactinium(IV) oxide	17
ICSD.201074	Complete	P3-M1	O3 Pu2	O3 Pu2	Plutonium(III) oxide - beta	15
ICSD.600447	Complete	IA3-	Cf2 O3	Cf2 O3	Californium sesquioxide	14
Pauling.531131	Complete	Ia-3	Cm2O3	Cm2O3		14
Pauling.531136	Complete	Ia-3	Bk2O3	Bk2O3		12
ICSD.622387	Complete	C12/M1	Cm2 O3	Cm2 O3	Curium sesquioxide	11
ICSD.26673	Complete	PM3-M	O3 U1	O3 U1	Uranium(VI) oxide - II	11
ICSD.24621	Complete	FM3-M	O1 Pa1	O1 Pa1	Protactinium oxide (1/1)	11
Pauling.531132	Complete	P-3m1	Cm2O3	Cm2O3		9
ICSD.28136	Complete	P6-2M	O8 U3	O8 U3	Triuranium octaoxide	9
ICSD.24906	Complete	CMCM	O8 U3	O8 U3	Triuranium octaoxide - beta	8
Pearson.559910	Complete	Fddd	O3U	UO3		8
Pauling.458644	Complete	C12/m1	Cf2O3	Cf2O3		7
Pauling.1301779	Complete	Ia-3	O3Pu2	Pu2O3		7
Pauling.1250860	Complete	I-43d	O9U4	U4O9		7
Pauling.1500041	Complete	Fm-3m	CmO	CmO		7
ICSD.31715	Complete	FM3-M	O1 Pu1	O1 Pu1	Plutonium(II) oxide	7
Pauling.1250669	Complete	I41/amd	O3U	UO3		6
ICSD.16756	Complete	C222	O8 U3	O8 U3	Uranium oxide (3/8)	6
ICSD.43809	Complete	FM3-M	Am1 O1	Am1 O1	Americium oxide (1/1)	6
ICSD.29333	Complete	PNMA	O5 U2	O5 U2	Uranium(V) oxide - delta	6
ICSD.261663	Complete	IMMM	O168 U32	O168 U32	Uranium oxide(I) (32/168)	6
ICSD.609784	Complete	P3-M1	Am2 O3	Am2 O3	Americium oxide (2/3)	5
ICSD.31628	Complete	P3-M1	O3 U1	O3 U1	Uranium(VI) oxide - alpha	5
ICSD.24223	Complete	FM3-M	O1 U1	O1 U1	Uranium(II) oxide	5
ICSD.15567	Complete	C2MM	O3 U1	O3 U1	Uranium(VI) oxide - alpha	5
ICSD.38146	Complete	P3-	O8 U3	O8 U3	Uranium diuranium(VI) oxide - high temperature modification	4
ICSD.31750	Complete	P3-M1	Ac2 O3	Ac2 O3	Actinium oxide	4
ICSD.26585	Complete	IA3-	Am2 O3	Am2 O3	Americium sequioxide	4
					m(II) oxide	4
					xide (13/34)	4
					) oxide - beta	4
						3

O Removal Energy of Actinide Oxides

- Save in a **structure list**:
  - 56 Ce/actinide oxide compounds in various space groups

MedeA: structure list editor

File Add structure(s) Display Properties QT: QSAR Toolbox

SQLite structure list file (72704 bytes): /home/rshan/MD/Structures/custom/actinide_oxides.sli
Containing 56 structure(s)

View structures from: 1 to: 56 Apply

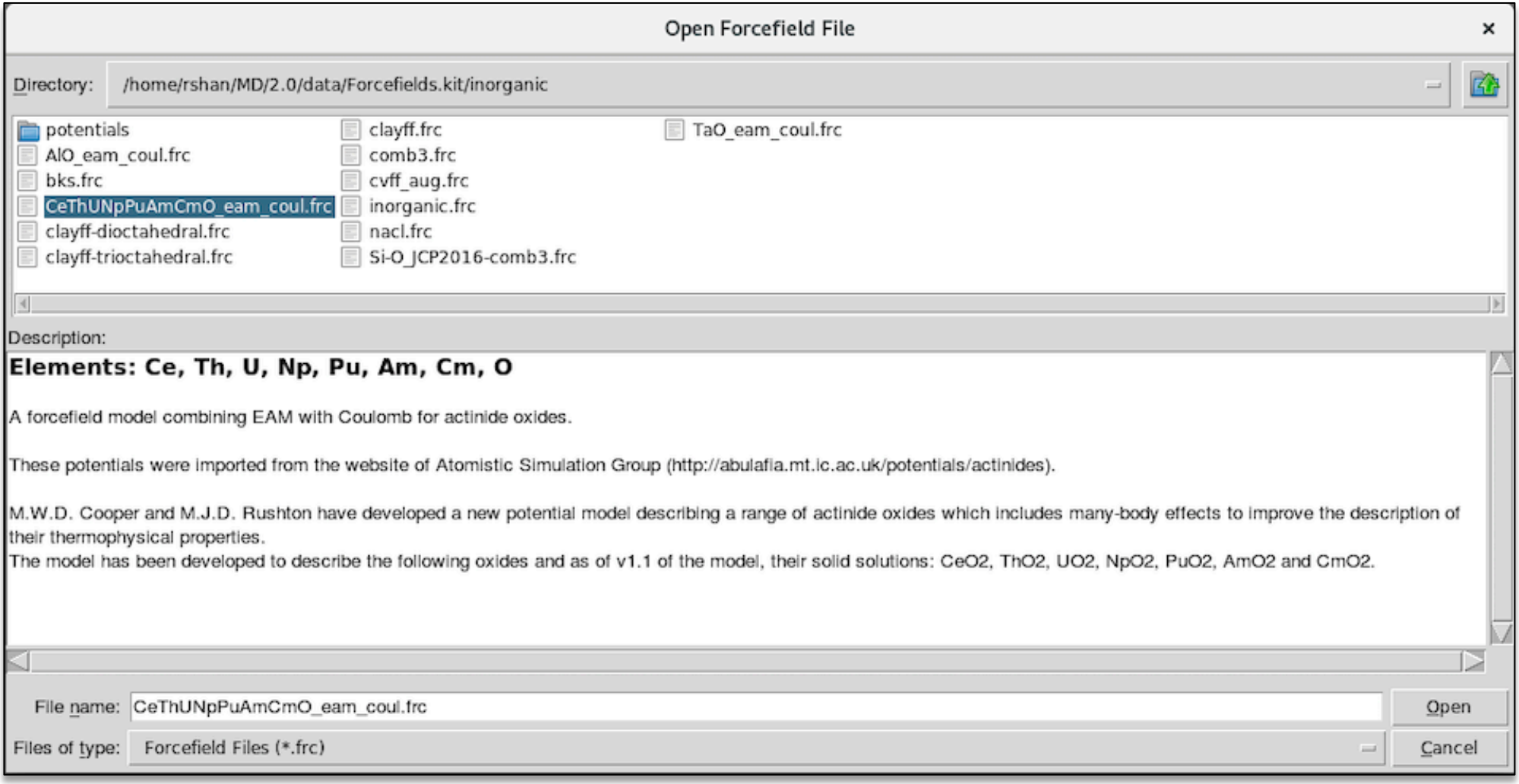
Structures Properties

Order	Name	Structural Formula	# atoms	# configurations	Symmetry	Cell parameters
1	Pearson.1620184	Am2O3	5	1	P-3m1	3.817 3.817 5.971 90 90 120
2	Pearson.535095	Am4O4	8	1	Fm-3m	5.045 5.045 5.045 90 90 90
3	ICSD.43810: Americium(IV) oxide	Am4O8	12	1	Fm-3m	5.378 5.378 5.378 90 90 90
4	Pearson.535091	Am12O18	30	1	C2/m	14.38 3.52 8.92 90 100.4 90
5	Pearson.1620183	Am32O48	80	1	Ia-3	11.03 11.03 11.03 90 90 90
6	Pearson.1711209	Ce2O3	5	1	P321	3.88 3.88 6.06 90 90 120
7	Pearson.260391	Ce2O3	5	1	P-3m1	3.891 3.891 6.059 90 90 120
8	ICSD.169031: Cerium dioxide - rutile-type, unstable	Ce2O4	6	1	P42/MNM	5.13 5.13 3.58 90 90 90
9	ICSD.189288: Cerium dioxide	Ce2O4	6	1	I4/mmm	2.321 2.321 5.754 90 90 90
10	ICSD.189287: Cerium dioxide	Ce2O4	6	1	P-3m1	3.214 3.214 4.025 90 90 120
11	Pearson.1301474	Ce4O4	8	1	Fm-3m	5.089 5.089 5.089 90 90 90
12	COD.7217887: Cerium(IV)oxide	Ce4O8	12	1	P1	5.3623 5.3623 5.3623 90 90 90
13	Pearson.1946553	Ce4O8	12	1	Fm-3m	5.411 5.411 5.411 90 90 90
14	Pearson.1639026	Ce4O8	12	1	Pnma	5.641 3.481 6.647 90 90 90
15	ICSD.88754: Cerium oxide (7/12)	Ce7O12	19	1	R-3R	6.785 6.785 6.785 99.42 99.42 99.42
16	ICSD.164744: Cerium(IV) oxide	Ce8O16	24	1	P1	7.72477 7.72477 5.46228 90 90 90
17	COD.1521460: Ce11 O20	Ce11O20	31	1	P-1	6.757 10.26 6.732 90.04 99.8 96.22
18	ICSD.160221: Cerium oxide - B	Ce12O18	30	1	C12/M1	14.785 3.7946 9.231 90 100.066 90
19	Pearson.1805252	Ce21O36	57	1	R-3	10.339 10.339 9.628 90 90 120
20	Pearson.556985	Ce32O48	80	1	Ia-3	11.26 11.26 11.26 90 90 90
21	Pearson.559956	Cm2O3	5	1	P-3m1	3.8 3.8 6 90 90 120
22	Pearson.1500041	Cm4O4	8	1	Fm-3m	5.026 5.026 5.026 90 90 90
23	Pearson.455758	Cm4O8	12	1	Fm-3m	5.36 5.36 5.36 90 90 90
24	ICSD.622387: Curium sesquioxide	Cm12O18	30	1	C12/M1	14.282 3.641 8.883 90 100.29 90
25	Pearson.458650	Cm21O36	57	1	R-3	10.1937 10.1937 9.4608 90 90 120
26	Pearson.531131	Cm32O48	80	1	Ia-3	11.0017 11.0017 11.0017 90 90 90
27	Pearson.451123	Np4O4	8	1	Fm-3m	5.01 5.01 5.01 90 90 90
28	Pearson.1943223	Np4O8	12	1	Fm-3m	5.453 5.453 5.453 90 90 90
29	Pearson.1623465	Np8O20	28	1	P2/c	8.168 6.584 9.313 90 116.09 90
30	COD.1530380: Pu2 O3	Pu2O3	5	1	P-3m1	3.8381 3.8381 5.918 90 90 120
31	Pearson.451120	Pu4O4	8	1	Fm-3m	4.958 4.958 4.958 90 90 90
32	Pearson.560118	Pu4O8	12	1	Fm-3m	5.397 5.397 5.397 90 90 90
33	Pearson.1301779	Pu32O48	80	1	Ia-3	11.0446 11.0446 11.0446 90 90 90
34	Pearson.383833	Th4O4	8	1	Fm-3m	5.302 5.302 5.302 90 90 90
35	Pearson.1831421	Th4O8	12	1	Fm-3m	5.597 5.597 5.597 90 90 90
36	Pearson.1907310	Th4O8	12	1	Pnma	5.898 3.6 6.862 90 90 90
37	ICSD.15567: Uranium(VI) oxide - alpha	U2O6	8	1	C2MM	3.961 6.86 4.166 90 90 90
38	Pearson.1250852	U3O8	11	1	P-3	6.815 6.815 4.136 90 90 120
39	Pearson.1125104	U3O8	11	1	P-62m	6.821 6.821 4.1517 90 90 120
40	Pearson.530900	U4O4	8	1	Fm-3m	4.92 4.92 4.92 90 90 90
41	ICSD.160813: Uranium oxide - HP	U4O8	12	1	Pa-3	5.329 5.329 5.329 90 90 90
42	Pearson.541856	U4O8	12	1	Fm-3m	5.47 5.47 5.47 90 90 90
43	Pearson.1250274	U4O12	16	1	P2_12_12_1	5.224 5.466 7.511 90 90 90
44	Pearson.1250855	U6O16	22	1	C222	6.704 11.95 4.142 90 90 90
45	Pearson.1250961	U6O16	22	1	Amm2	4.147 11.96 6.716 90 90 90
46	ICSD.160815: Uranium oxide - HP	U8O16	24	1	Pbca	9.688 5.332 5.35 90 90 90
47	COD.2310373: U O3	U10O30	40	1	P1211	10.34 14.33 3.91 90 99.03 90
48	Pearson.1250856	U12O32	44	1	P2_1/m	6.72 8.29 11.93 90 91 90
49	Pearson.1250154	U12O32	44	1	Cmcm	7.069 11.445 8.303 90 90 90
50	COD.1529146: Li2 (U3 O10)	U12O40	52	1	P121/c1	6.821 18.91 7.3 90 121.56 90
51	Pearson.1250669	U16O48	64	1	I4_1/amd	6.9013 6.9013 19.9754 90 90 90

Close

O Removal Energy of Actinide Oxides

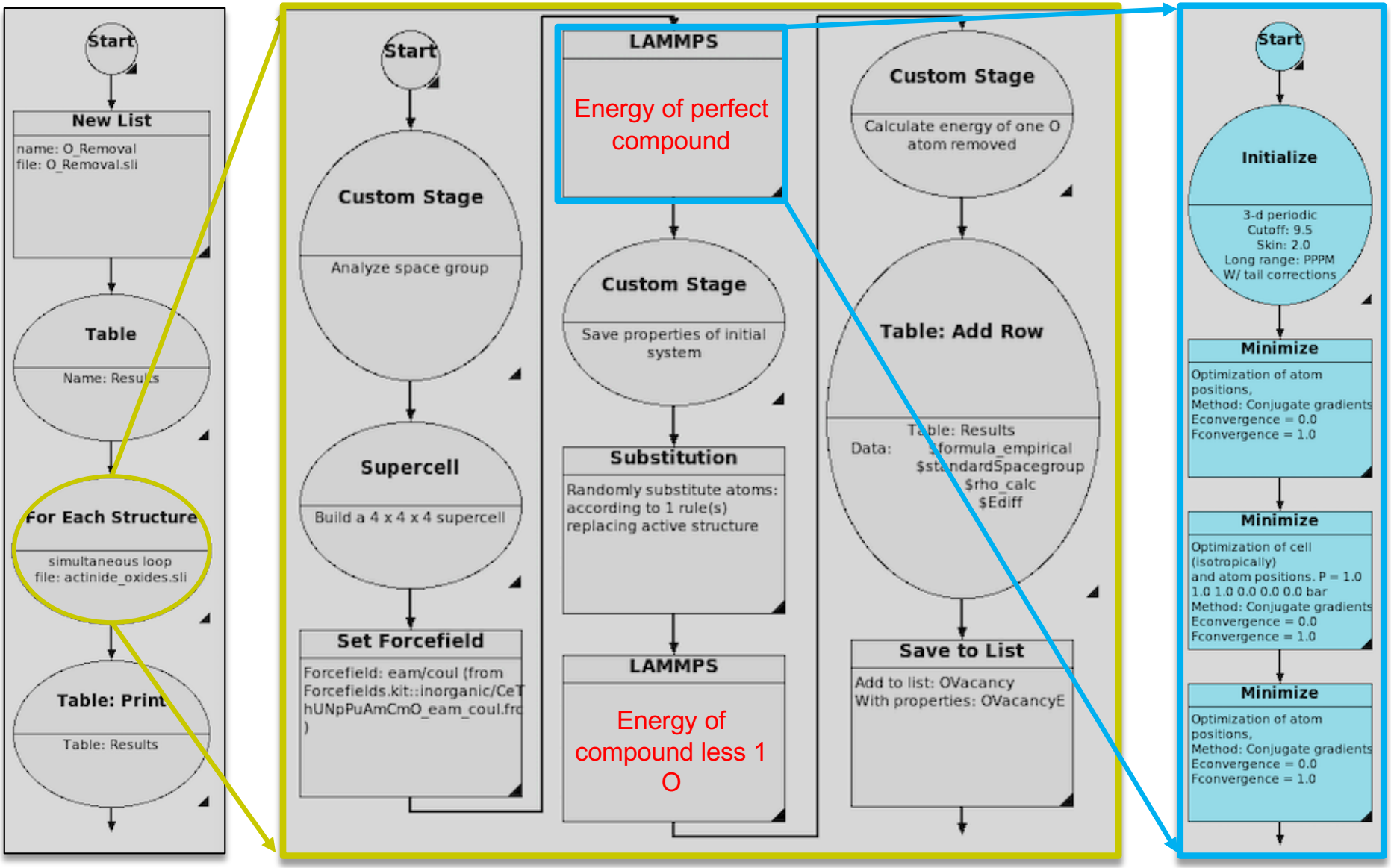
- Assign the Cooper force field for actinide oxides [1]



[1] http://abulafia.mt.ic.ac.uk/potentials/actinides

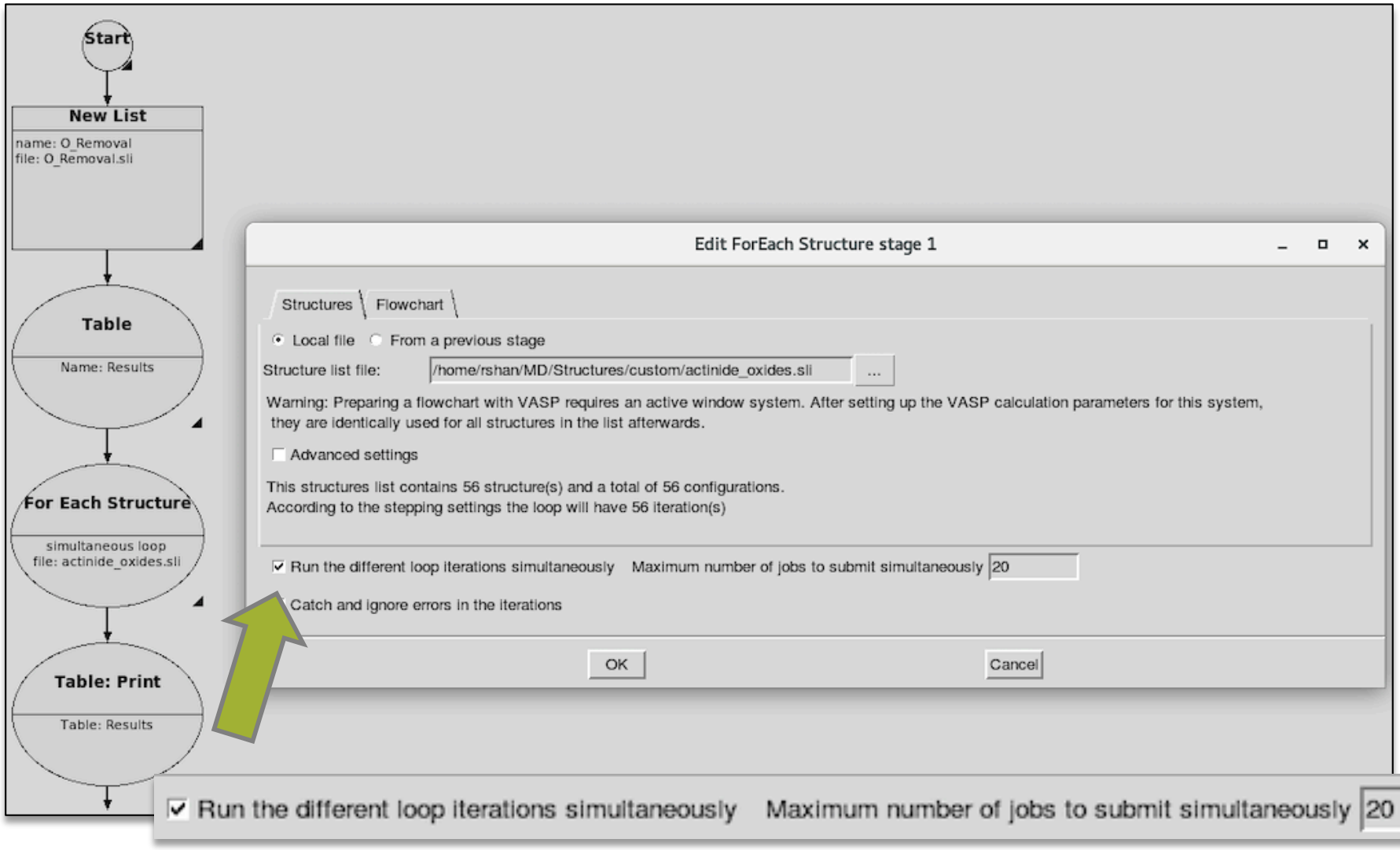
O Removal Energy of Actinide Oxides

- Prepare a High-throughput flowchart



Run HT calculations in parallel or serial

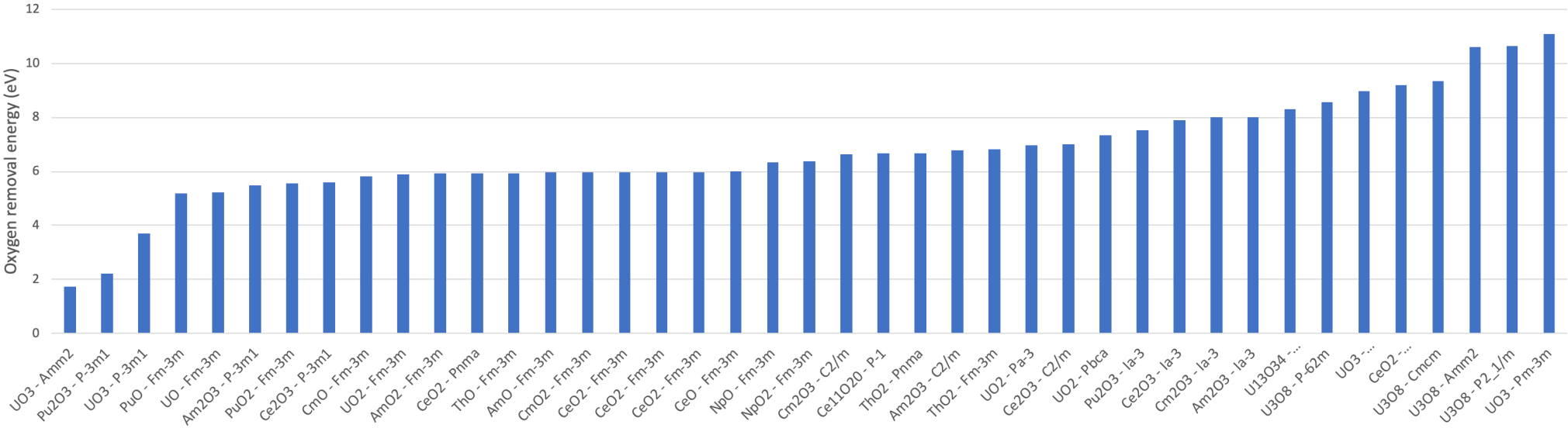
- Value: Highly efficient screening of large number of compounds



O Removal Energy of Actinide Oxides

- View results from Job.out
  - 112 (56*2) calculations finished in 749 seconds on an 8-core Intel Linux box

Formula	Space Group	Density g/cm^3	OVacancyEnergy eV
Am2O3	P-3m1	13.5234	2.063400
AmO	Fm-3m	15.2106	5.953601
AmO2	Fm-3m	11.8527	5.917101
Am2O3	C2/m	13.3225	7.237001
Am2O3	Ia-3	12.2707	8.011002
Ce2O3	P321	4.4884	-732.879751
Ce2O3	P-3m1	8.1413	3.246101
CeO2	P4_2/mnm	6.3383	9.205002
CeO2	I4/mmm	7.9265	-115.379024
CeO2	P-3m1	8.2788	-33.889407
CeO	Fm-3m	8.9324	5.996101
CeO2	Fm-3m	7.2611	5.981401
U3O8	P-62m	7.3755	8.549902
UO	Fm-3m	14.6722	5.218701
UO2	Pa-3	10.4769	6.975001
UO2	Fm-3m	11.0449	5.903401
UO3	P2_12_12_1	8.3340	8.101002
U3O8	Amm2	7.3810	10.619602
UO2	Pbca	10.9016	7.341002
UO3	P2_1	8.0113	-148.610031
U3O8	P2_1/m	7.2044	7.213001
U3O8	Cmcm	7.1665	10.653002
UO3	I4_1/amd	7.4985	-125.429026
U13O34	Amm2	7.2381	8.780002
UO3	P-3m1	7.6785	3.683401
UO3	Pm-3m	5.4056	11.080502



- Can further convert O removal energy to O vacancy formation energy by considering energy of O_2

Summary

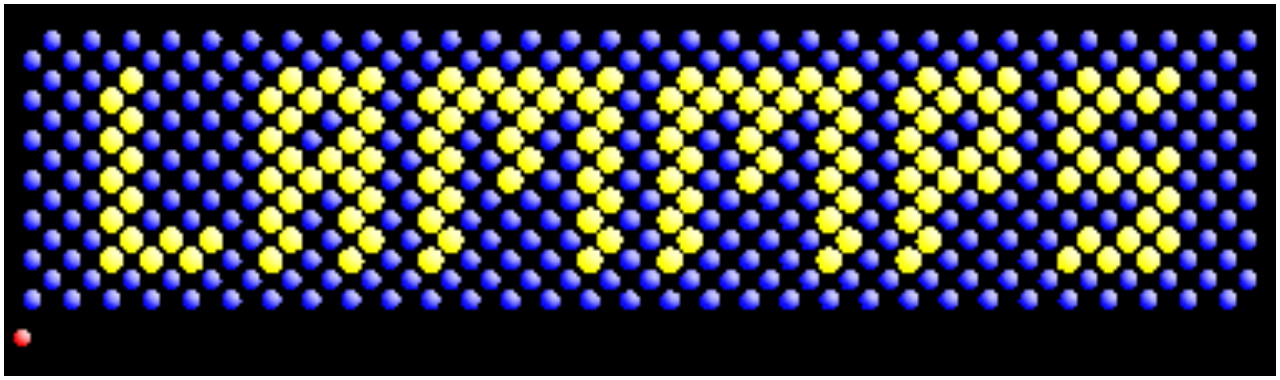
- Screened 56 Ce/O, Am/O, Cm/O, Np/O, Pu/O, Th/O, and U/O compounds for their oxygen removal energies
  - Directly imported structures from MedeA® databases to structure list
  - Set up LAMMPS calculations with Cooper potential
  - Results written to a table and a csv text file
- Same flowchart and strategy can be applied to other materials properties using other potentials

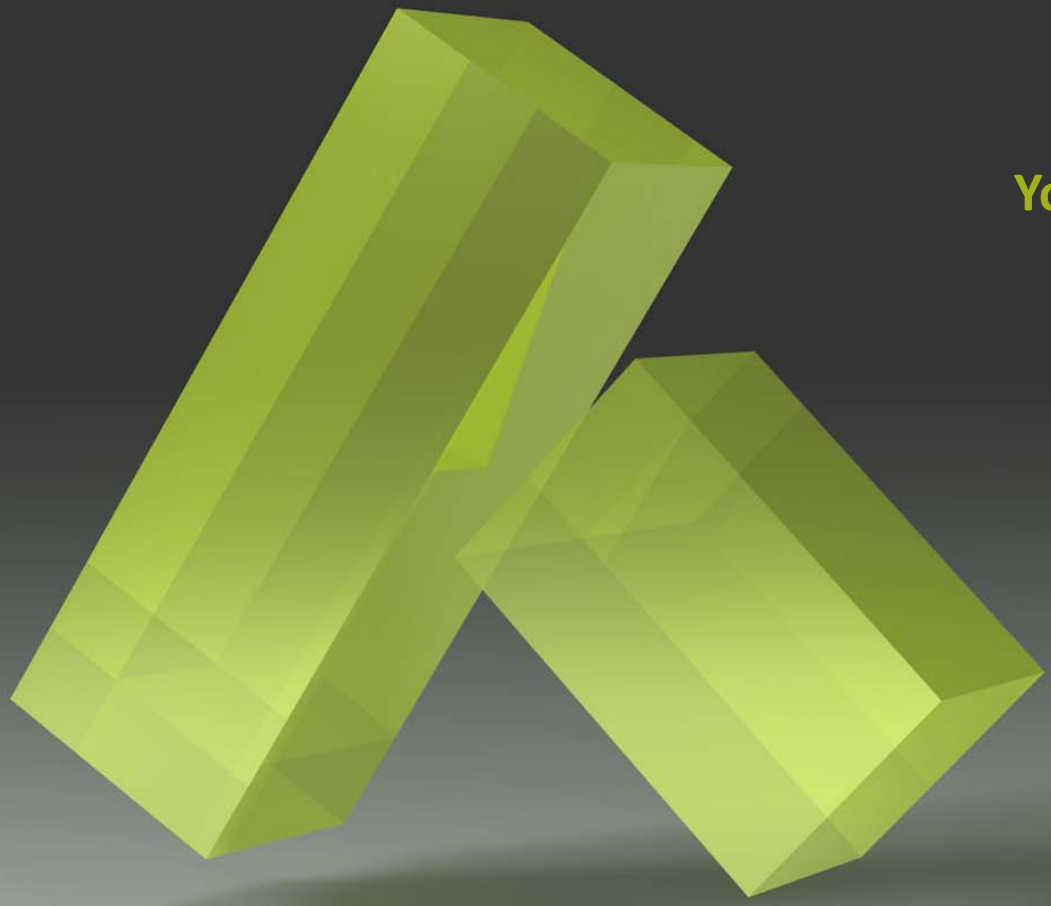
Conclusions

- The MedeA® environment hosts a variety of versatile tools required for creation of realistic models of materials
  - Molecules, amorphous liquids and solids
  - Bulk polymer, crosslinked resins
  - Interfacial systems and composites
- Integration of highly regarded simulation codes, including LAMMPS, VASP, GIBBS, MOPAC, and Gaussian enables multiple types of property calculation on materials of interest.
- MedeA® High Throughput Launchpad enables the automated, massive screening, exploring, and sampling of materials properties
  - Young's modulus of thermoset resins
  - Oxygen removal energy of actinide oxides

Acknowledgements

- Aidan Thompson, Steve Plimpton, and Stan Moore





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