



materials design

Calculs à Haut Débit dans l'Environnement Logiciel *MedeA*

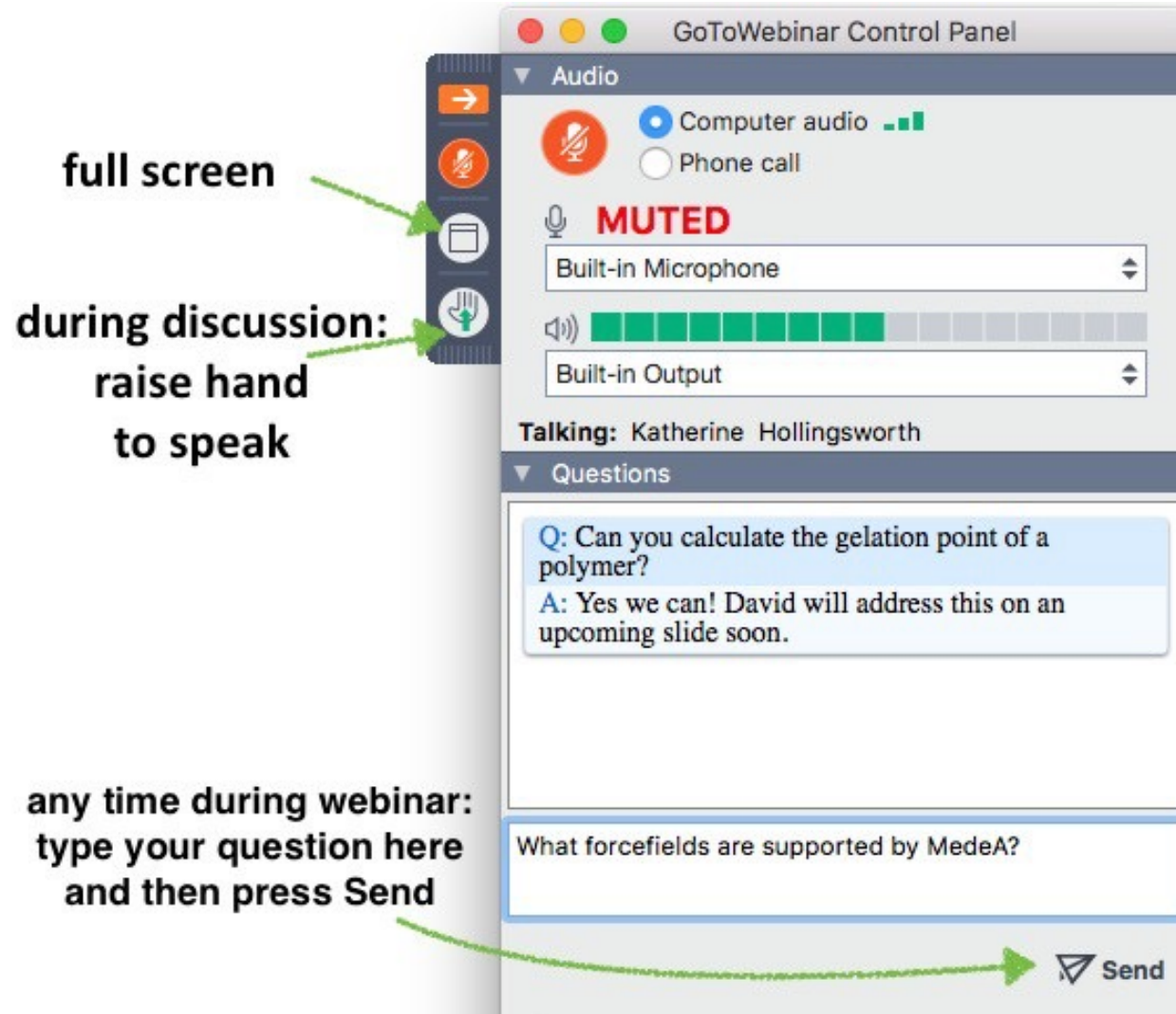
Materials Design, SARL
Juin 2021



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The screenshot shows the GoToWebinar Control Panel interface. On the left, a vertical toolbar contains several icons: a right-pointing arrow, a microphone with a slash, a hand icon, and a hand with a raised index finger. Annotations with green arrows point to these icons: 'full screen' points to the right-pointing arrow; 'during discussion: raise hand to speak' points to the hand with a raised index finger icon. The main panel is divided into sections: 'Audio' with 'Computer audio' selected and 'MUTED' status; 'Talking: Katherine Hollingsworth'; and 'Questions' with a Q&A exchange. A text input field at the bottom contains the question 'What forcefields are supported by MedeA?' and a 'Send' button with a paper plane icon. A green arrow points from the text 'any time during webinar: type your question here and then press Send' to the 'Send' button.

full screen

**during discussion:
raise hand
to speak**

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

GoToWebinar Control Panel

Audio

Computer audio Phone call

MUTED

Built-in Microphone

Built-in Output

Talking: Katherine Hollingsworth

Questions

Q: Can you calculate the gelation point of a polymer?

A: Yes we can! David will address this on an upcoming slide soon.

What forcefields are supported by MedeA?

Send



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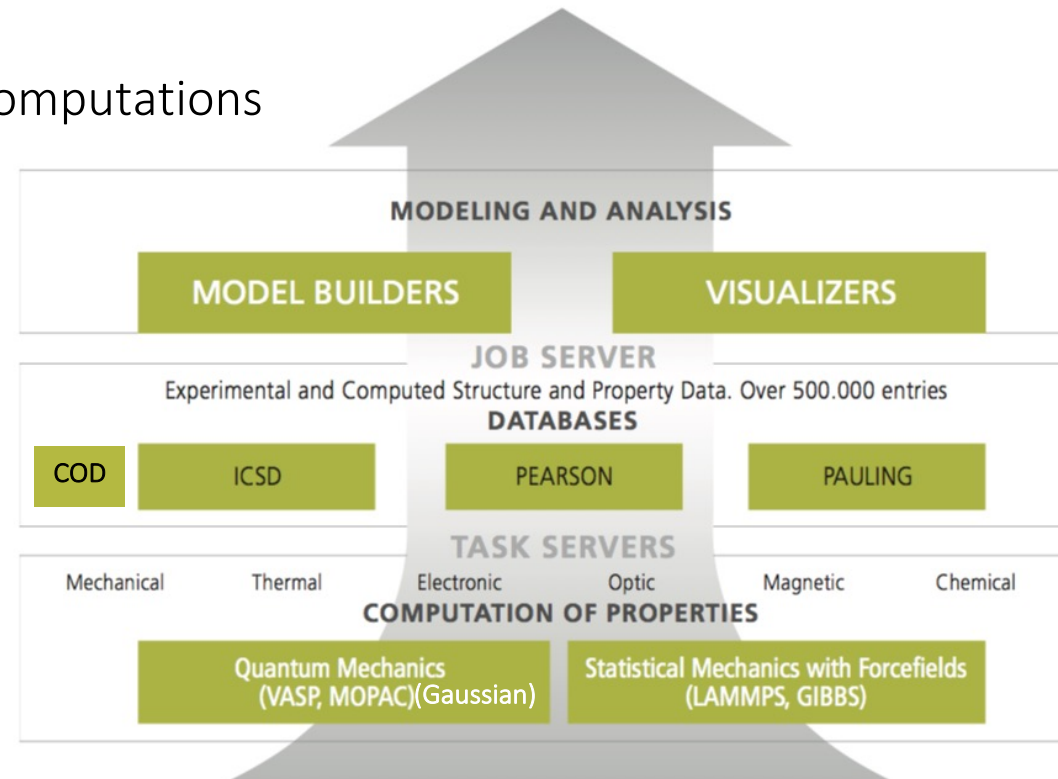
materials design

Calculs à Haut Débit dans l'Environnement Logiciel *MedeA*

Materials Design, SARL
Juin 2021

Environnement Logiciel *MedeA*

- ▶ Data central in *MedeA*
 - Integrating of experimental data with simulations
 - currently > 1 M data entries + computed data
- ▶ Fast technology development
 - High-throughput data generation by experiment and computations
 - Data storage and handling
 - Cloud computing
 - Massive parallelization
- ▶ Big data: Novel approaches for exploiting data
 - Neural networks, deep learning, machine learning

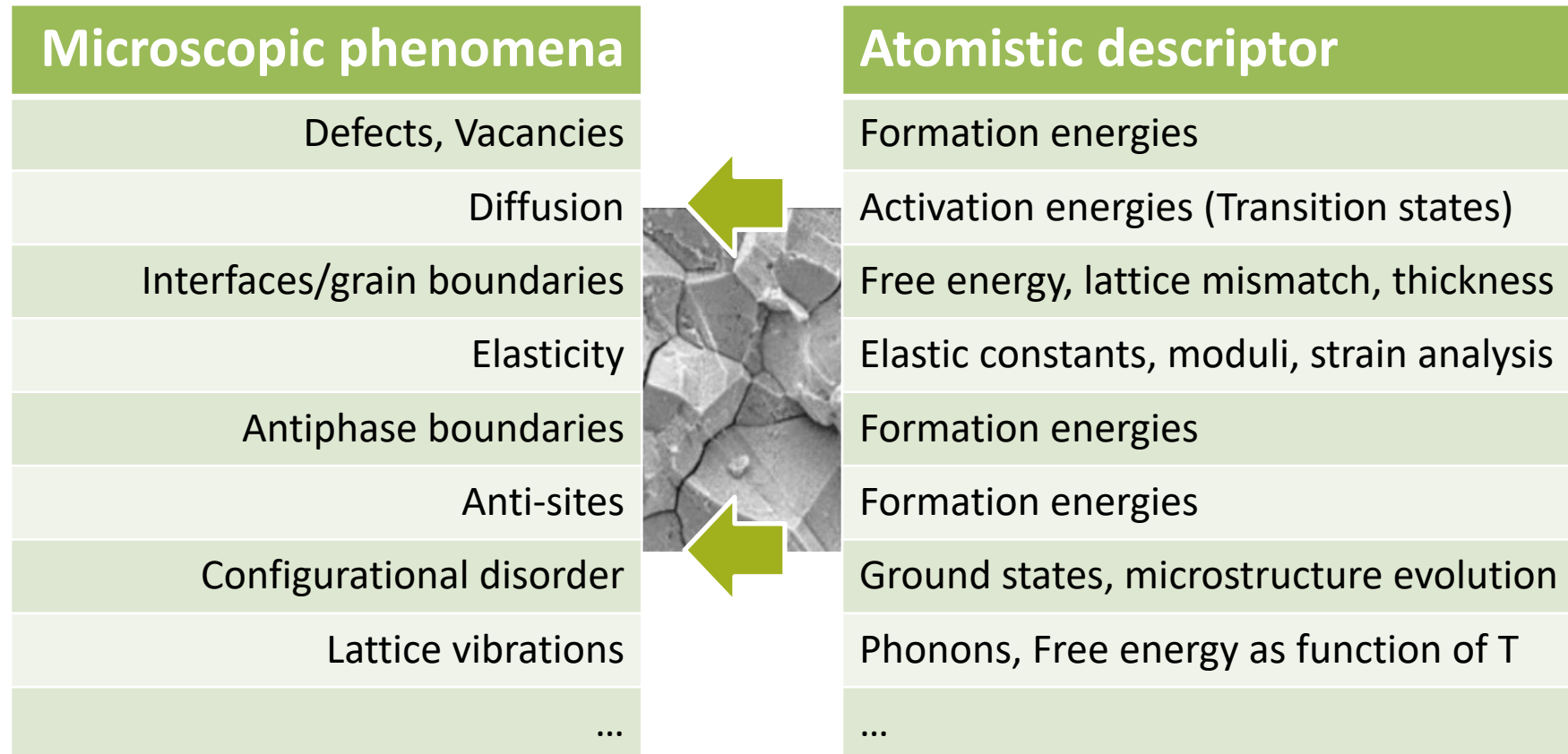




Échantillonnage et Statistique

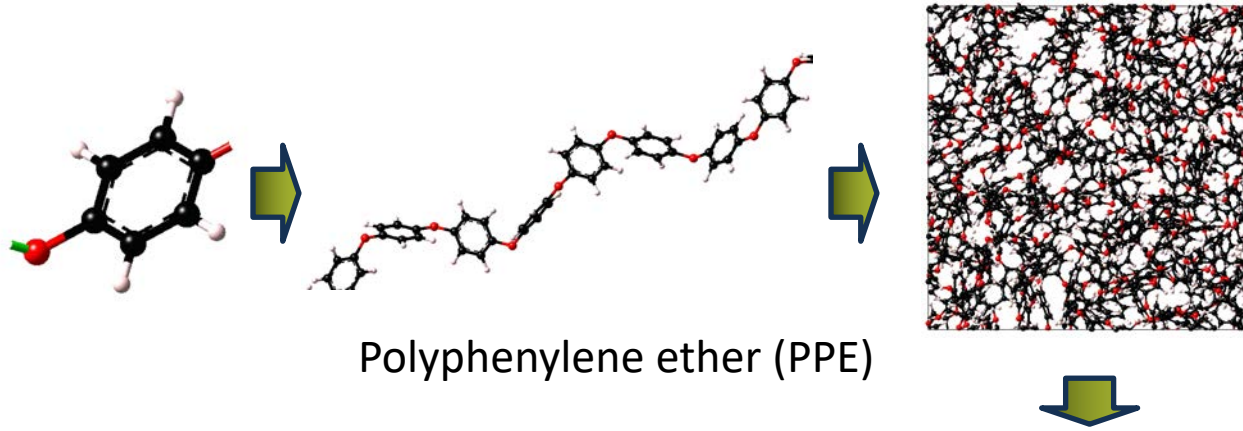


Les propriétés des matériaux découlent de phénomènes microscopiques



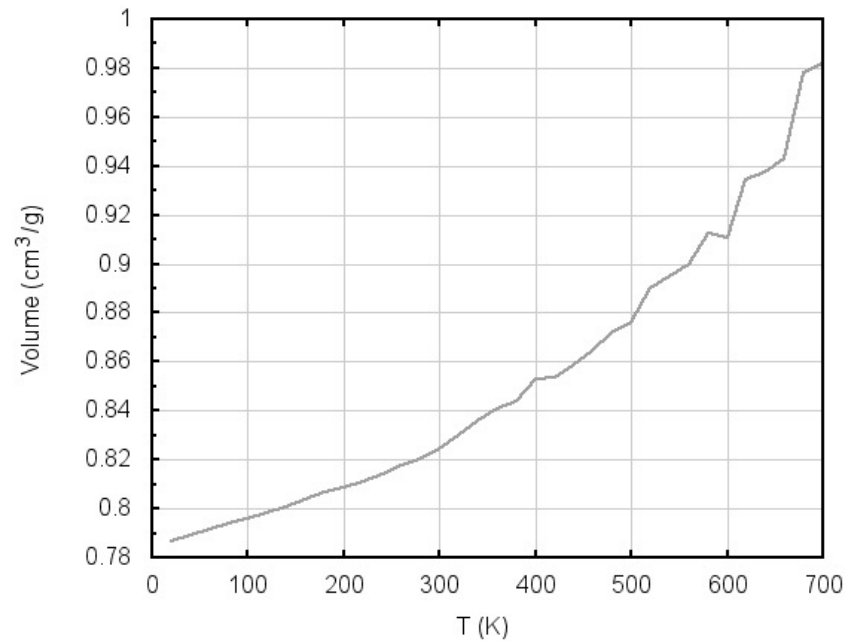


Température de Transition Vitreuse (T_g) d'un Polymère



Polyphenylene ether (PPE)

Volume vs Temperature Analysis

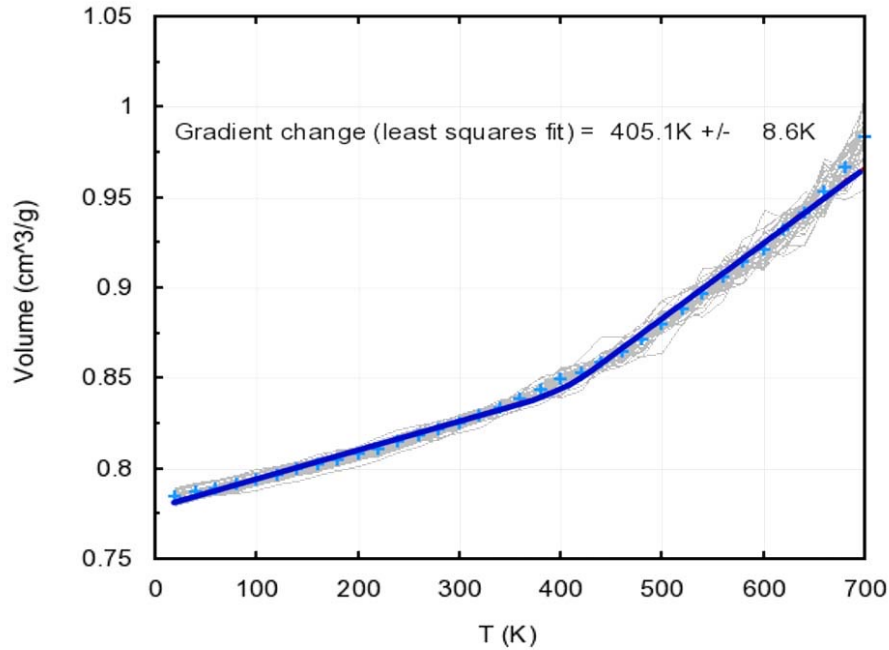


Where is the transition?



Température de Transition Vitreuse (T_g) d'un Polymère

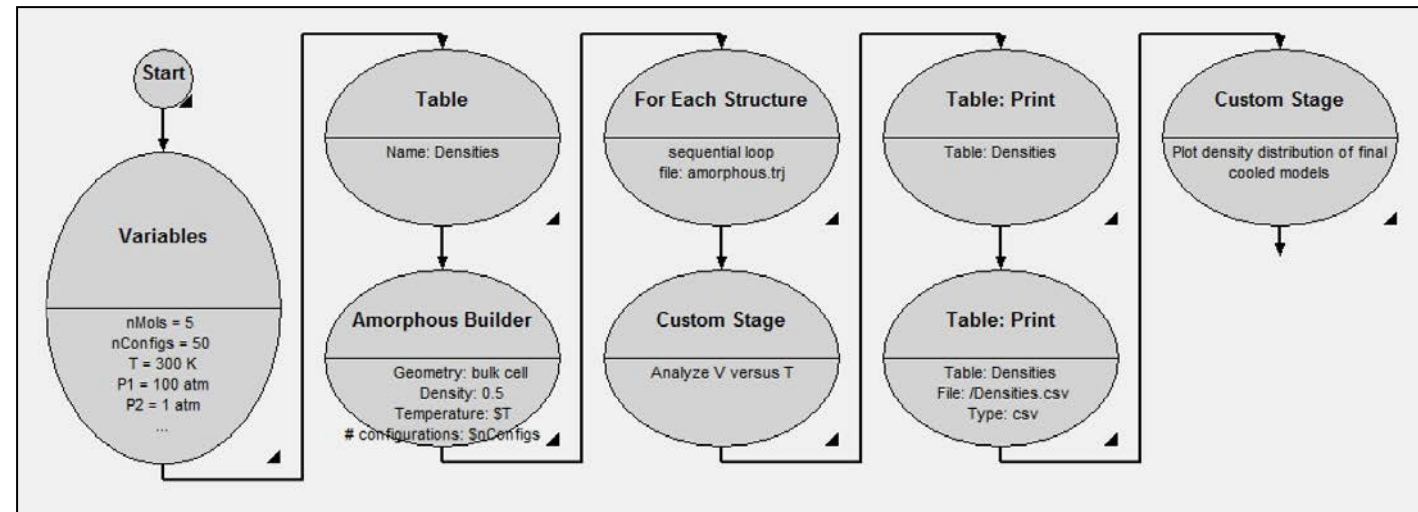
Volume vs Temperature Analysis



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





Échantillonnage des Propriétés Mécaniques de Résines Thermodurcissables

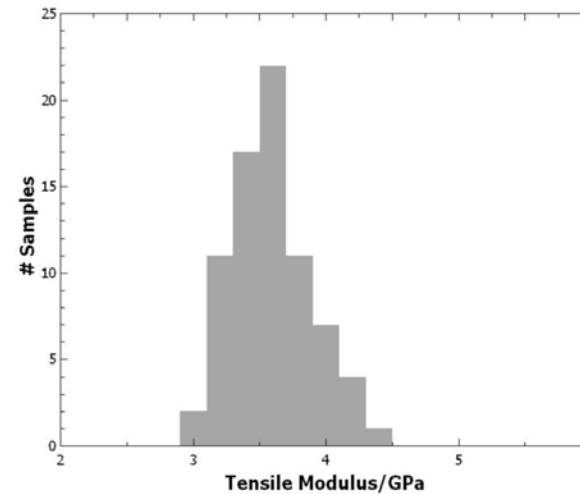
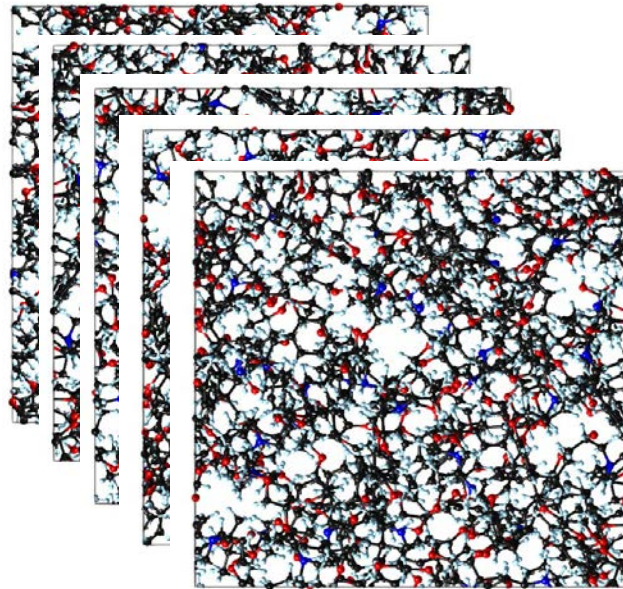


Figure 12. Distribution of tensile moduli of a batch of crosslinked DGEBA-DDS thermoset models.

Resin	Calculated (GPa)	Experiment (GPa)	Ref.
DGEBA	3.49-3.53	$2.4 \pm .15$ - $3.2 \pm .15$	17
TGAP	4.42-4.45	$4.396 \pm .027$	18
TGDDM	5.18-5.19	$5.103 \pm .033$	18

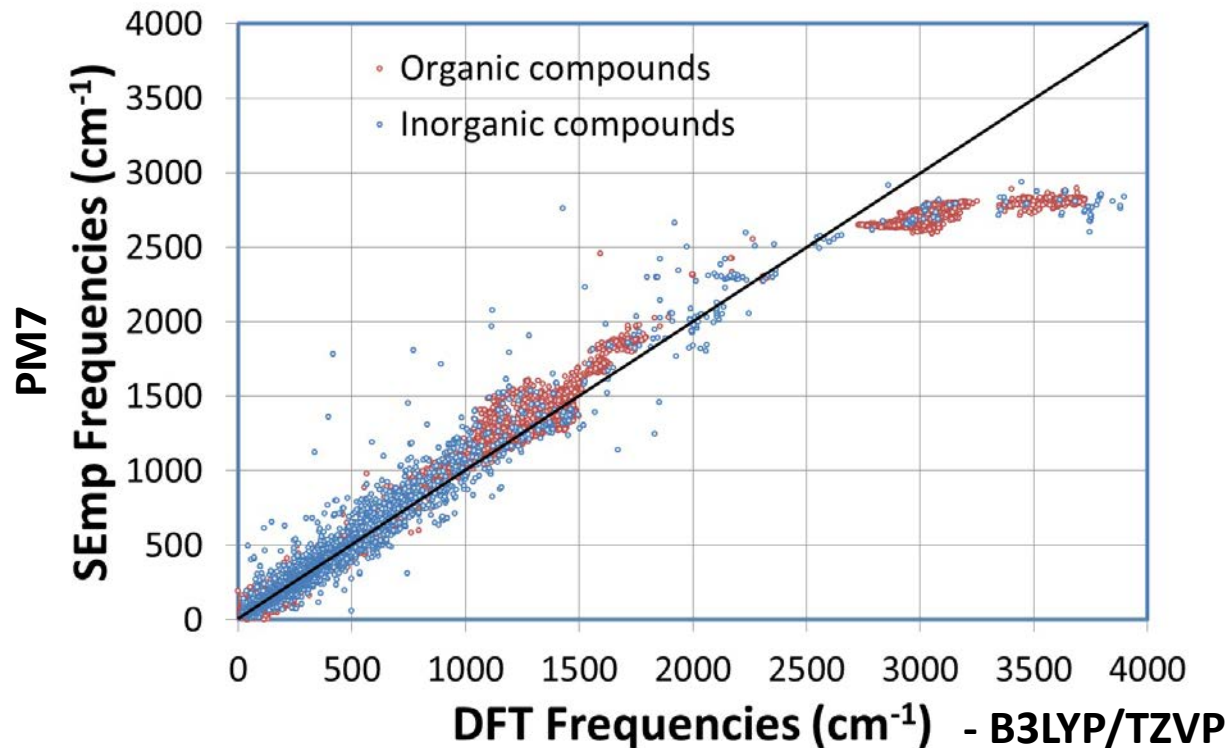
Table 1. Comparison of calculated and experimentally-measured tensile moduli for epoxy resins based on di, tri and tetrafunctional resin architectures.

From: Rigby, D., et al, 2014. Computational prediction of mechanical properties of glassy polymer blends and thermosets. In Advanced Composites for Aerospace, Marine, and Land Applications (pp. 157-171). Springer International Publishing.



Validation Méthodologique – Comparaison Systématique

- ▶ Comparison between the vibrational frequencies computed with semi-empirical and DFT methods for organic and inorganic molecules: 1395 molecules, ~42,000 frequencies



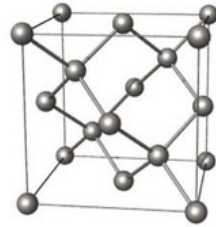
Rozanska *et al.* *J. Chem. Eng. Data* **2014**, *59*, 3136-3143 & *Oil Gas Sci. Tech.* **2015**, *70*, 405-417



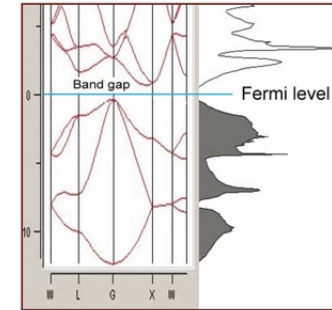
Calculs à Haut Débit

Calculs à Haut Débit

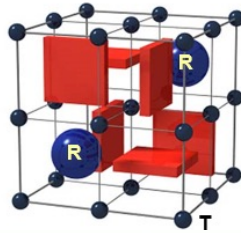
Serial



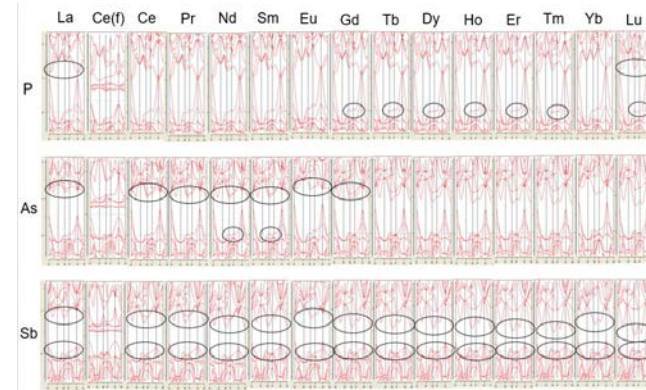
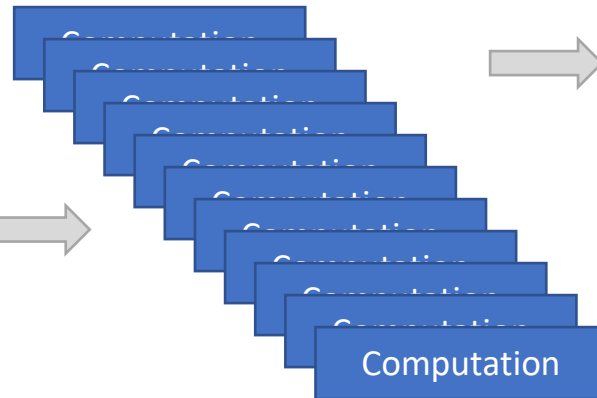
Computation



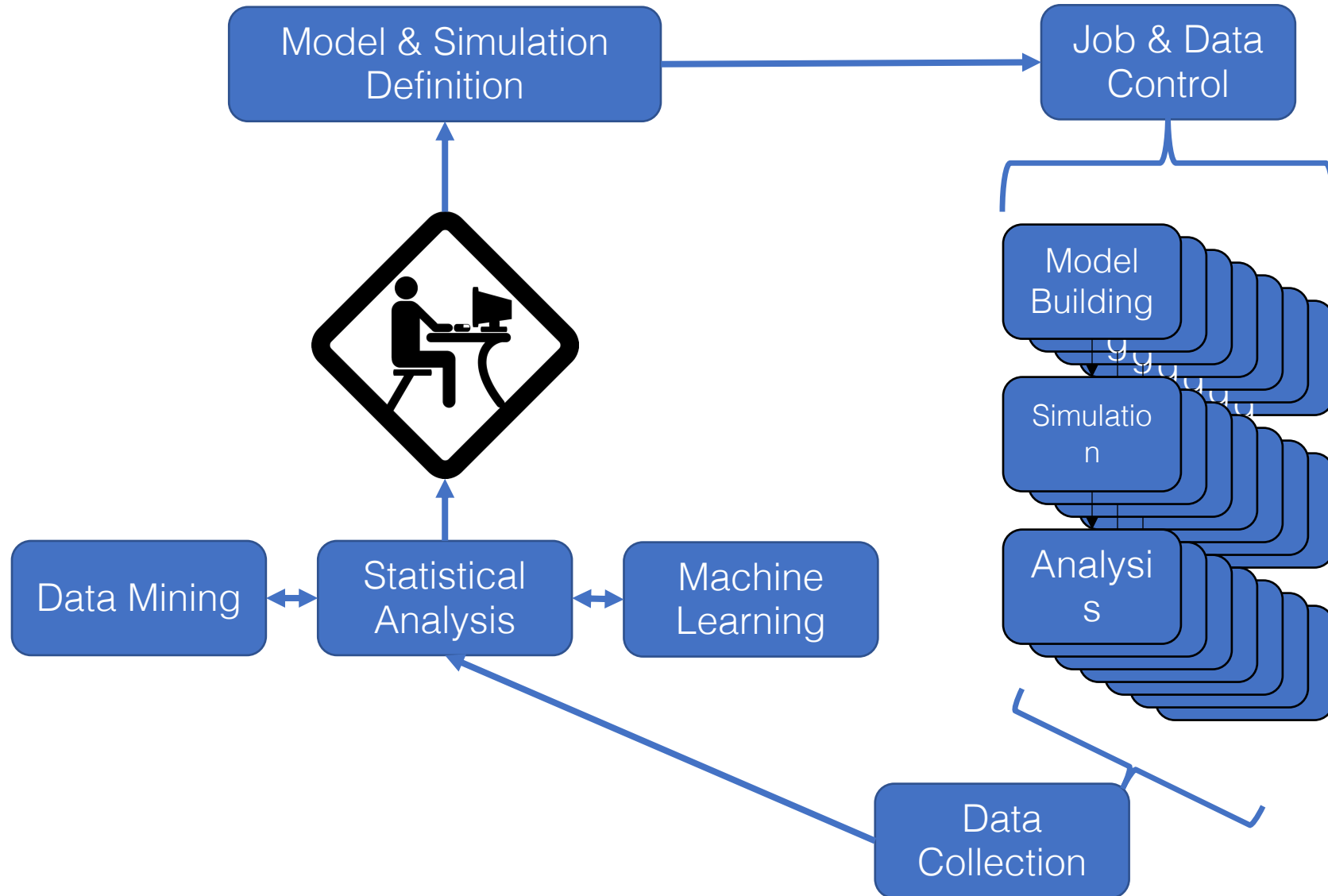
High Throughput



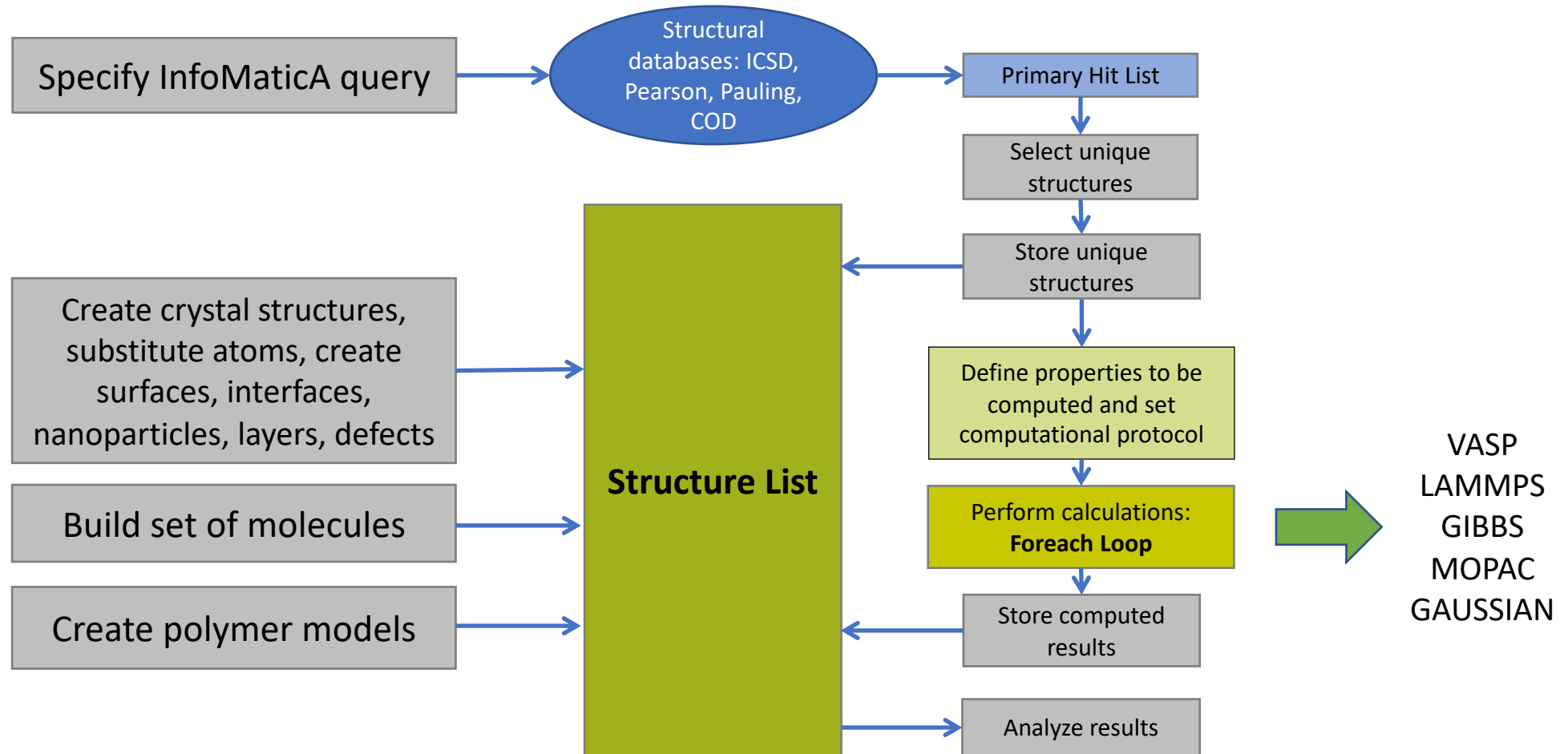
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H																	He
2	Li	Be											B	C	N	O		Ne
3	Na	Mg											Al	Si	P	S	Cl	Ar
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Cu	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Ra	Ac	Rf	Ha	Sg	Nh	Mc											
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		



Flux des Tâches



Mise en Œuvre du Calcul Haut Débit dans *MedeA*

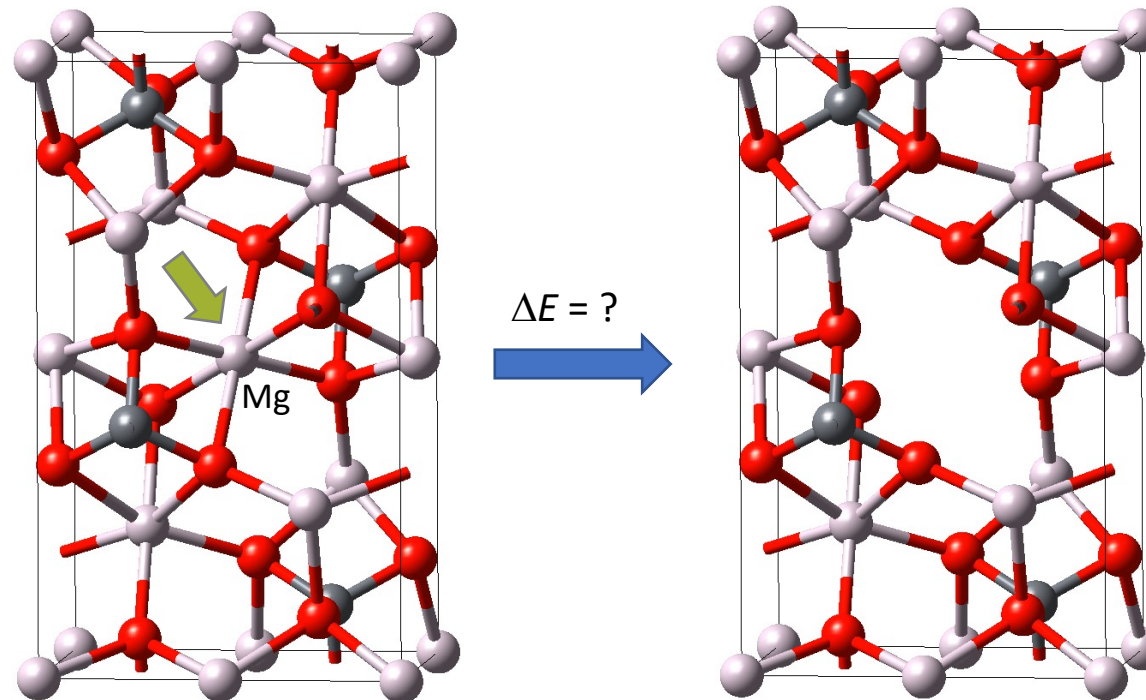




Un Calcul à Haut Débit en Pratique

Énergies de Liaison d'Atome de Magnésium

- ▶ How strongly is Mg bonded in known Mg-containing compounds?





Exemple d'une Recherche dans les Bases de Données Cristallographiques avec l'Outil *InfoMaticA* de *MedeA*

► Querying InfoMaticA for Mg containing compounds, with fewer than 6 elements, and a unit cell volume less than 2000\AA^3

Search Criteria | Detailed Information | Coordinates | Geometry | Coordination | Pair Correlation | Powder pattern

Require that formula contains any number of atoms of Mg

Require that number of elements is less than 6

Require that volume is less than 2000.0

Require that structural completeness complete

Require that --Add new criterion--

Run search Clear

Displaying 0 of 0 hits



Résultats de la Recherche

Materials Design: InfoMaticA -- Search

ID	completeness	space group name H-M	sum	structural	name systematic
ICSD.609872	Complete	P3-M1	As2 Be2 Mg1	As2 Be2 Mg1	Magnesium beryllium arsenide (1/2/2)
ICSD.260394	Complete	PNMA	H6 Mg2 Na2 Ni1	H6 Mg2 Na2 Ni1	Sodium magnesium hydride tetrahydronicolate (2/2/2/1)
ICSD.260406	Complete	PNMA	D6 Mg2 Na2 Ni1	D6 Mg2 Na2 Ni1	Dimagnesium disodium nickel hexadeuteride
ICSD.83779	Complete	FD3-MS	Mg2 O4 Si1	Mg2 O4 Si1	Magnesium silicate - spinel
ICSD.83780	Complete	FD3-MS	Mg2 O4 Si1	Mg2 O4 Si1	Magnesium silicate - spinel
ICSD.260407	Complete	PNMA	H6 Mg2 Na2 Ni1	H6 Mg2 Na2 Ni1	Dimagnesium disodium nickel hexadeuteride
ICSD.31106	Complete	PBNM	Ca1 Mg1 O4 Si1	Ca1 Mg1 O4 Si1	Calcium magnesium silicate
ICSD.83781	Complete	FD3-MS	Mg2 O4 Si1	Mg2 O4 Si1	Magnesium silicate - spinel
ICSD.5007	Complete	P321	Al1 F6 Li1 Mg1	Al1 F6 Li1 Mg1	Lithium magnesium hexafluoroaluminate
ICSD.184412	Complete	P63/MMC	Mg1 Zn2	Mg1 Zn2	Magnesium zinc (1/2)
ICSD.164171	Complete	PBNM	Fe1 Mg1 O4 Si1	Fe1 Mg1 O4 Si1	Iron magnesium silicate
ICSD.83782	Complete	FD3-MS	Mg2 O4 Si1	Mg2 O4 Si1	Magnesium silicate - spinel
ICSD.5008	Complete	PNMA	D3 K1 Mg1 N2	D3 K1 Mg1 N2	potassium magnesium deuterio-imide deuterio-diamide
ICSD.164172	Complete	PBNM	Fe1 Mg1 O4 Si1	Fe1 Mg1 O4 Si1	Iron magnesium silicate
ICSD.83783	Complete	FD3-MS	Mg2 O4 Si1	Mg2 O4 Si1	Magnesium silicate - spinel
ICSD.164173	Complete	PBCA	Fe1 Mn1 O6 Si2	Fe1 Mn1 O6 Si2	Iron magnesium catena-disilicate

Search Criteria | Detailed Information | Coordinates | Geometry | Coordination | Pair Correlation | Powder pattern

Require that contains any number of

Require that is less than

Require that is less than

Require that

Require that

Run search Clear

Displaying 500 of 4368 hits

- 4368 database entries returned

Élimination des Structures Redondantes

'Find median structures' command retains representative structures...

The screenshot shows the Materials Design software interface. A search results table is displayed with columns: space group name H-M, sum, structural, and name systematic. A context menu is open over the table, with 'Find median structures' highlighted. Below the table, search criteria are defined: formula contains any number of atoms of Mg, number of elements is less than 6, volume is less than 2000.0, and structural completeness is complete. A 'Median' button is visible. A scatter plot on the right shows cell length a (Ang) vs Entry #.

ICSD	Complete	space group name H-M	sum	structural	name systematic
ICSD.83779	Complete	P3-M1	As2 Be2 Mg1	As2 Be2 Mg1	Magnesium beryllium arsenide (1/2/2)
ICSD.83780	Complete	PNMA	H6 Mg2 Na2 Ni1	H6 Mg2 Na2 Ni1	Sodium magnesium hydride tetrahydridonicolate (2/2/2/1)
ICSD.260407	Complete	PNMA	D6 Mg2 Na2 Ni1	D6 Mg2 Na2 Ni1	Dimagnesium disodium nickel hexadeuteride
ICSD.31106	Complete	PBNM	Mg2 O4 Si1	Mg2 O4 Si1	Magnesium silicate - spinel
ICSD.83781	Complete	FD3-MS	Mg2 O4 Si1	Mg2 O4 Si1	Magnesium silicate - spinel
ICSD.5007	Complete	P321	H6 Mg2 Na2 Ni1	H6 Mg2 Na2 Ni1	Dimagnesium disodium nickel hexadeuteride
ICSD.184412	Complete	P63/MMC	Ca1 Mg1 O4 Si1	Ca1 Mg1 O4 Si1	Calcium magnesium silicate
ICSD.164171	Complete	PBNM	Mg2 O4 Si1	Mg2 O4 Si1	Magnesium silicate - spinel
ICSD.83782	Complete	FD3-MS	Al1 F6 Li1 Mg1	Al1 F6 Li1 Mg1	Lithium magnesium hexafluoroaluminate
ICSD.5008	Complete	PNMA	Mg1 Zn2	Mg1 Zn2	Magnesium zinc (1/2)
ICSD.164172	Complete	PBNM	Fe1 Mg1 O4 Si1	Fe1 Mg1 O4 Si1	Iron magnesium silicate
ICSD.83783	Complete	FD3-MS	Fe1 Mg1 O4 Si1	Fe1 Mg1 O4 Si1	Iron magnesium silicate
ICSD.164173	Complete	PBCA	D3 K1 Mg1 N2	D3 K1 Mg1 N2	potassium magnesium deuterio-imide deuterio-diamide
			Fe1 Mg1 O4 Si1	Fe1 Mg1 O4 Si1	Iron magnesium silicate
			Mg2 O4 Si1	Mg2 O4 Si1	Magnesium silicate - spinel
			Fe1 Mg1 O6 Si2	Fe1 Mg1 O6 Si2	Iron magnesium catena-disilicate

Search Criteria: Detailed Information | Coordinates | Geometry | Coordination | Pair Correlation | Powder pattern

Require that formula contains any number of atoms of Mg

Require that number of elements is less than 6

Require that volume is less than 2000.0

Require that structural completeness complete

Require that --Add new criterion--

Run search Clear

Find median structure for each formula and spacegroup in the table

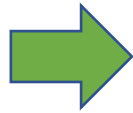
Median

cell length a (Ang)

Entry #

↳ Liste de Structures Réduite

This yields 1443 structures for further analysis and computation



Materials Design: InfoMaticA -- Search

ID	completeness	space group name H-M	sum	structural	name systematic
ICSD.262083	Complete	P42NM	H8 B2 Mg1	H8 B2 Mg1	Magnesium bis(tetrahydridoborate) - HP phase
COD.9007818	Complete	P42mc	Cl2 Mg O10	Mg(ClO2)2.6H2O	
COD.2013721	Complete	P12/m1	C10 H16 Mg O14	C10 H16 Mg O14	hexaaquamagnesium(II) benzene-1,2,4,5-tetracarboxylate(2-)
ICSD.417035	Complete	P12/M1	Co2 Gd4 Mg3	Co2 Gd4 Mg3	Tetragadolinium trimagnesium dicobalt
ICSD.416490	Complete	P12/M1	Co2 Mg3 Nd4	Co2 Mg3 Nd4	Neodymium cobalt magnesium (4/2/3)
ICSD.416491	Complete	P12/M1	Co2 Mg3 Sm4	Co2 Mg3 Sm4	Samarium cobalt magnesium (4/2/3)
ICSD.417036	Complete	P12/M1	Co2 Mg3 Tb4	Co2 Mg3 Tb4	Tetraerbium trimagnesium dicobalt
ICSD.190935	Complete	P112/M	H2 Mg1 O4 Si1	H2 Mg1 O4 Si1	Magnesium dihydrogen silicate
ICSD.27533	Complete	P12/M1	Mg2 O4 Si1	Mg2 O4 Si1	Magnesium silicate - model I
ICSD.419312	Complete	P4-21M	Ba2 Ge2 Mg1 O7	Ba2 Ge2 Mg1 O7	Dibarium magnesium digermanate
ICSD.81117	Complete	P4-21M	Ba2 Mg1 O7 Si2	Ba2 Mg1 O7 Si2	Dibarium magnesium disilicate
ICSD.50065	Complete	P4-21M	Ca2 Mg1 O7 Si2	Ca2 Mg1 O7 Si2	Dicalcium magnesium disilicate
ICSD.261224	Complete	P4-21M	Eu2 Mg1 O7 Si2	Eu2 Mg1 O7 Si2	Europium magnesium disilicate
ICSD.420522	Complete	P4-21M	Ge2 Mg1 O7 Sr2	Ge2 Mg1 O7 Sr2	Distrontium magnesium digermanate
ICSD.261226	Complete	P4-21M	Mg1 O7 Si2 Sr2	Mg1 O7 Si2 Sr2	Distrontium magnesium disilicate

Search Criteria | Detailed Information | Coordinates | Geometry | Coordination | Pair Correlation | Powder pattern

Require that formula contains any number of atoms of Mg

Require that number of elements is less than 6

Require that volume is less than 2000.0

Require that structural completeness complete

Require that --Add new criterion--

▶ 1443 structures

Run search Clear

Displaying 500 of 1443 hits

Revue des Données de la Liste de Structures

Each entry provides additional information on the structure: i.e. source, geometry, symmetry, atomic coordinates, etc.

The screenshot shows the Materials Design: InfoMaticA search interface. The main window displays a table of search results with columns for ID, completeness, space group name H-M, sum, structural, and name systematic. A green arrow points from the text on the left to the 'Detailed Information' tab of the selected entry, ICSD.262083.

ID	completeness	space group name H-M	sum	structural	name systematic
ICSD.262083	Complete	P42NM	H8 B2 Mg1	H8 B2 Mg1	Magnesium bis(tetrahydridoborate) - HP phase
COD.9007818	Complete	P42mc	Cl2 Mg O10	Mg(ClO2)2.6H2O	
COD.2013721	Complete	P12/m1	C10 H16 Mg O14	C10 H16 Mg O14	hexaaquamagnesium(II) benzene-1,2,4,5-tetracarboxylate(2-)
ICSD.417035	Complete	P12/M1	Co2 Gd4 Mg3	Co2 Gd4 Mg3	Tetragadolinium trimagnesium dicobalt
ICSD.416490	Complete	P12/M1	Co2 Mg3 Nd4	Co2 Mg3 Nd4	Neodymium cobalt magnesium (4/2/3)
ICSD.416491	Complete	P12/M1	Co2 Mg3 Sm4	Co2 Mg3 Sm4	Samarium cobalt magnesium (4/2/3)
ICSD.417036	Complete	P12/M1	Co2 Mg3 Tb4	Co2 Mg3 Tb4	Tetraerbium trimagnesium dicobalt
ICSD.190935	Complete	P112/M	H2 Mg1 O4 Si1	H2 Mg1 O4 Si1	Magnesium dihydrogen silicate
ICSD.27533	Complete	P12/M1	Mg2 O4 Si1	Mg2 O4 Si1	Magnesium silicate - model I
ICSD.419312	Complete	P4-21M	Ba2 Ge2 Mg1 O7	Ba2 Ge2 Mg1 O7	Dibarium magnesium digermanate
ICSD.81117	Complete	P4-21M	Ba2 Mg1 O7 Si2	Ba2 Mg1 O7 Si2	Dibarium magnesium disilicate
ICSD.50065	Complete	P4-21M	Ca2 Mg1 O7 Si2	Ca2 Mg1 O7 Si2	Dicalcium magnesium disilicate
ICSD.261224	Complete	P4-21M	Eu2 Mg1 O7 Si2	Eu2 Mg1 O7 Si2	Europium magnesium disilicate
ICSD.420522	Complete	P4-21M	Ge2 Mg1 O7 Sr2	Ge2 Mg1 O7 Sr2	Distrontium magnesium digermanate
ICSD.261226	Complete	P4-21M	Mg1 O7 Si2 Sr2	Mg1 O7 Si2 Sr2	Distrontium magnesium disilicate

Detailed Information | Coordinates | Geometry | Coordination | Pair Correlation | Powder pattern

ICSD.262083 MgB₂H₈

H8 B2 Mg1
Magnesium bis(tetrahydridoborate) - HP phase

Symmetry

Spacegroup: **P42NM** Z: **2.**
SpGrp Number: Volume: **181.65**
Pearson symbol: **tP22** Calculated density:

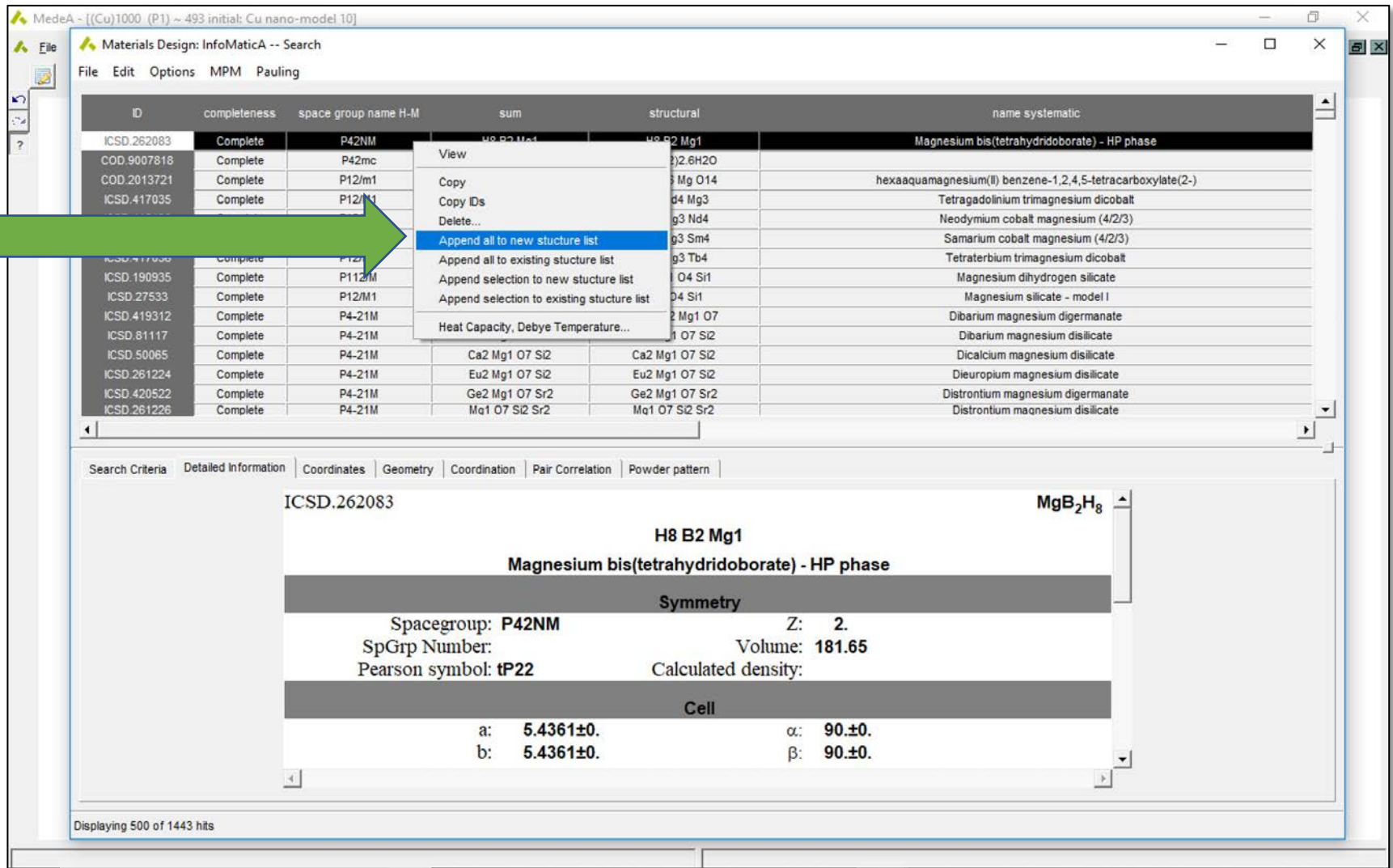
Cell

a: **5.4361±0.** α: **90.±0.**
b: **5.4361±0.** β: **90.±0.**

Displaying 500 of 1443 hits

Sauvegarde de la Liste de Structures

The refined list is saved directly as a structure list



The screenshot shows the Materials Design software interface. The top window displays a search results table with columns: ID, completeness, space group name H-M, sum, structural, and name systematic. A context menu is open over the first row (ICSD.262083), with the option 'Append all to new structure list' highlighted. A green arrow points from the text on the left to this menu item. Below the table, the 'Detailed Information' tab is selected, showing the following details for ICSD.262083:

ICSD.262083 MgB₂H₈

H8 B2 Mg1
Magnesium bis(tetrahydridoborate) - HP phase

Symmetry

Spacegroup: **P42NM** Z: 2.
SpGrp Number: Volume: 181.65
Pearson symbol: **tP22** Calculated density:

Cell

a: 5.4361±0.	α: 90.±0.
b: 5.4361±0.	β: 90.±0.

Displaying 500 of 1443 hits



Liste de Structures

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

SQLite structure list file (1620992 bytes): C:/Users/clive/Desktop/MagnesiumCompoundsNew.sli
Containing 1443 structure(s)

View structures from: to:

Structures Properties

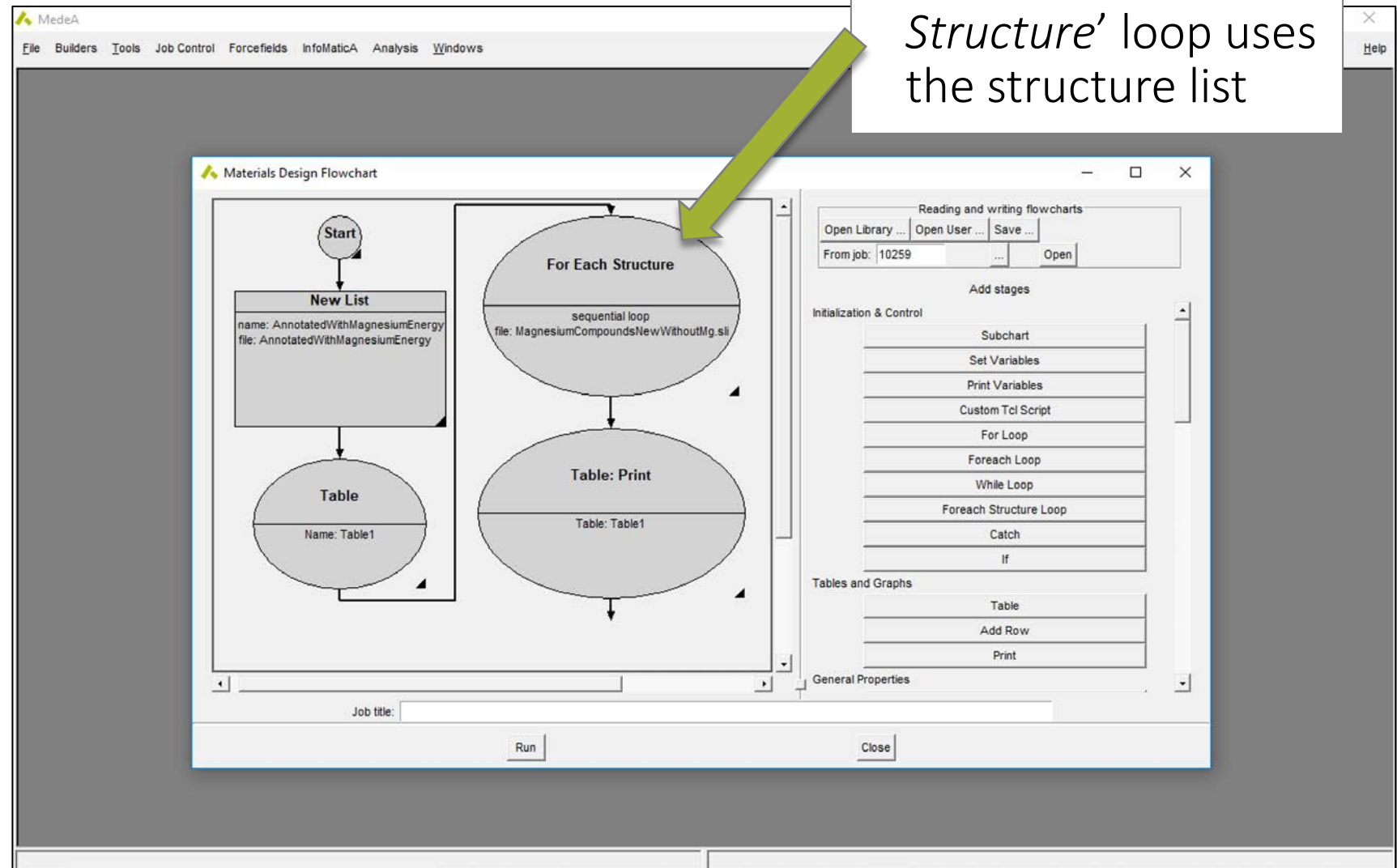
Order	Name	Structural Formula	# atoms	# configurations	Symmetry	Cell parameters
1	ICSD.262083: Magnesium bis(tetrahydridoborate) - HP phase	Mg2B4H16	22	1	P42Nm	5.4361 5.4361 6.1468 90 90 90
2	COD.9007818	Mg2Cl4O20	26	1	P42mc	7.471 7.471 9.98 90 90 90
3	COD.2013721: hexaaquamagnesium(II) benzene-1,2,4,5-tetracarboxylate(2-)	MgC10O14H16	41	1	P12/m1	6.447 9.942 6.455 90 115.148 90
4	ICSD.417035: Tetragadolinium trimagnesium dicobalt	Gd4Co2Mg3	9	1	P12/M1	7.54 3.741 8.225 90 109.65 90
5	ICSD.416490: Neodymium cobalt magnesium (4/2/3)	Nd4Co2Mg3	9	1	P12/M1	7.6542 3.8053 8.3247 90 109.79 90
6	ICSD.416491: Samarium cobalt magnesium (4/2/3)	Sm4Co2Mg3	9	1	P12/M1	7.6012 3.7711 8.2684 90 109.68 90
7	ICSD.417036: Tetraterbium trimagnesium dicobalt	Tb4Co2Mg3	9	1	P12/M1	7.504 3.7286 8.195 90 109.48 90
8	ICSD.190935: Magnesium dihydrogen silicate	MgSiO4H2	8	1	P112/M	4.756 4.266 2.844 90 90 92.99
9	ICSD.27533: Magnesium silicate - model I	Mg8Si4O16	28	1	P12/M1	10.11 5.77 4.7 90 90 90
10	ICSD.419312: Dibarium magnesium digermanate	Ba4Mg2Ge4O14	24	1	P-421M	8.3667 8.3667 5.542 90 90 90
11	ICSD.81117: Dibarium magnesium disilicate	Ba4Mg2Si4O14	24	1	P-421M	8.2036 8.2036 5.4058 90 90 90
12	ICSD.50065: Dicalcium magnesium disilicate	Ca4Mg2Si4O14	24	1	P-421M	7.8338 7.8338 5.0082 90 90 90
13	ICSD.261224: Dieuropium magnesium disilicate	Eu4Mg2Si4O14	24	1	P-421M	8.0138 8.0138 5.1711 90 90 90
14	ICSD.420522: Distrontium magnesium digermanate	Sr4Mg2Ge4O14	24	1	P-421M	8.1725 8.1725 5.315 90 90 90
15	ICSD.261226: Distrontium magnesium disilicate	Sr4Mg2Si4O14	24	1	P-421M	8.0107 8.0107 5.1636 90 90 90
16	ICSD.51245: Magnesium chloride	MgCl2	3	1	P-4m2	4.06 4.06 4.188 90 90 90
17	ICSD.416341: Magnesium boride carbide (2/24/1)	Mg4B48C2	54	1	P-4n2	8.9391 8.9391 5.0745 90 90 90
18	ICSD.165651: Magnesium bis(tetrahydridoborate)	Mg4B8H32	44	1	I-4m2	8.18 8.18 9.965 90 90 90
19	ICSD.249592: Strontium magnesium indide (1/1/3)	Sr2Mg2In6	10	1	I-4m2	4.6895 4.6895 12.629 90 90 90
20	COD.4328859: ?	Nd26Mg4Si8B16O86	140	1	P121/m1	9.1691 15.8763 11.78 90 106.12 90
21	ICSD.30654: Trimagnesium manganese dimanganese(III) diborate	Mn6Mg6B4O20	36	1	P121/M1	5.36 5.98 12.73 90 120.57 90
22	COD.4118939: ?	Na6Mg2P2C2O14	26	1	P121/m1	8.82663 6.61646 5.15605 90 89.6919 90
23	ICSD.67816: Potassium manganese tetracopper trivanadium oxide	K2V6Cu8Mg2O26	44	1	P121/M1	10.7144 6.0282 8.3365 90 98.075 90
24	ICSD.94669: Strontium magnesium fluoride - II	Sr12Mg12F48	72	1	P1121/M	7.8249 7.493 16.9248 90 90 105.041
25	ICSD.78532: Sodium lanthanum magnesium tellurium(VI) oxide	Na2La2Mg2Te2O12	20	1	P121/M1	5.5526 5.5349 7.9126 90 90.22 90
26	ICSD.40497: Sodium lanthanum manganese tungsten oxide	Na2La2W2Mg2O12	20	1	P121/M1	5.5239 5.5253 7.8939 90 90.16 90
27	ICSD.150576: Magnesium zinc (1/2) - eta'	Mg2Zn4	6	1	P121/M1	4.97 5.54 4.97 90 120 90
28	COD.9010402	Mg6Si6O18	30	1	P121/m1	7.026 6.228 4.262 90 95.85 90
29	COD.9010401	Mg8Si8O24	40	1	P121/m1	9.477 6.205 4.256 90 98.75 90
30	ICSD.107151: Magnesium silicoantimonide	As16Mg16Si16	48	1	I-42	0.1761 0.1761 11.606 90 90 90

Close



Organigramme des Tâches du Calcul du Potentiel Chimique du Magnésium

- A 'For Each Structure' loop uses the structure list



⚡ Détails du Protocol du Calcul pour le Magnésium

- Core of the protocol : 2 VASP energy calculations

The screenshot displays the Medea software interface. The main window is titled 'Edit ForEach Structure stage 1' and shows a flowchart with the following steps:

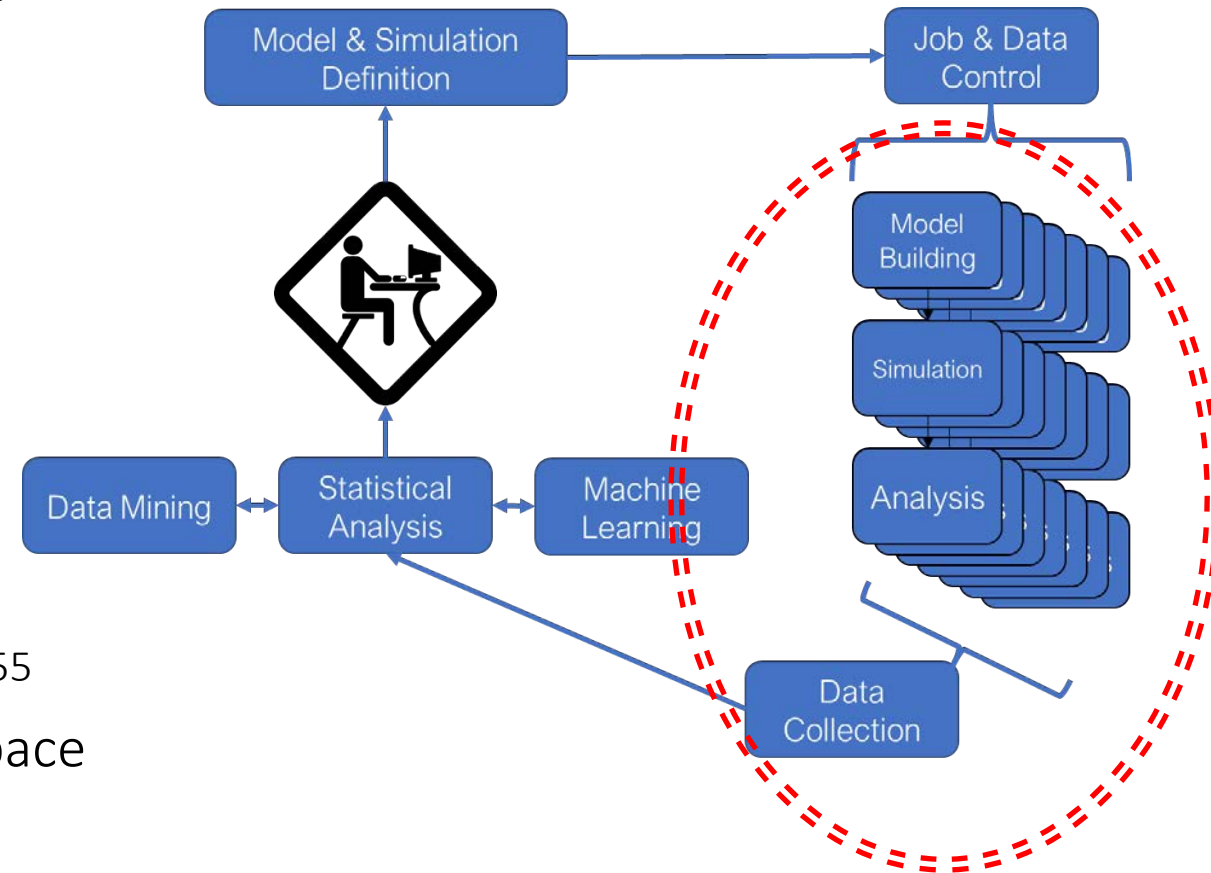
- Start
- Supercell (Build a 1 x 1 x 1 supercell)
- VASP
- Custom Stage (Save the initial electronic energy)
- Custom Stage (Delete a randomly selected magnesium atom)
- Custom Stage (Determine the energy required to remove a magnesium atom)
- VASP
- Table: Add Row (Table: Table1, Data: SeMgRemoval)
- Save to List (Add to list: AnnotatedWithMagnesiumEnergy, With properties: MagnesiumExtractionEnergy)

Below the flowchart, there are checkboxes for 'Run the different loop iterations simultaneously' (checked) and 'Catch and ignore errors in the iterations'. A green arrow points to the 'OK' button, which is circled in yellow. Another green arrow points to the 'Submit Run job' dialog box in the bottom left corner, which has the following settings:

- Queue: ContractMontrouge
- Number of processors: 16
- Priority: 5
- Buttons: Run, Cancel

Quels sont les Tâches dans l'Organigramme?

- ▶ Provides visual protocol & summary of the calculation steps
- ▶ Manages the computations for 1443 structures
 - Uses (only) 16 cores *
 - In this case, runs for 8.9 days (local hardware)
 - Carries out 2886 VASP calculations
 - Transfers and manages ~63,000 files
 - Collects results for permanent storage
 - Let you examine all calculations details
- ▶ Prepares a report summarizing results
- ▶ Provides a unique identifier for sharing results
 - E.g. http link <http://1.2.3.4:32000/jobStatus.tml?id=10155>
- ▶ Allowing you to survey efficiently parameter space



*) using 1600 cores all these calculations would have taken about 3 hours.



Liste de Structures Obtenue aprèS Calculs

Computed property

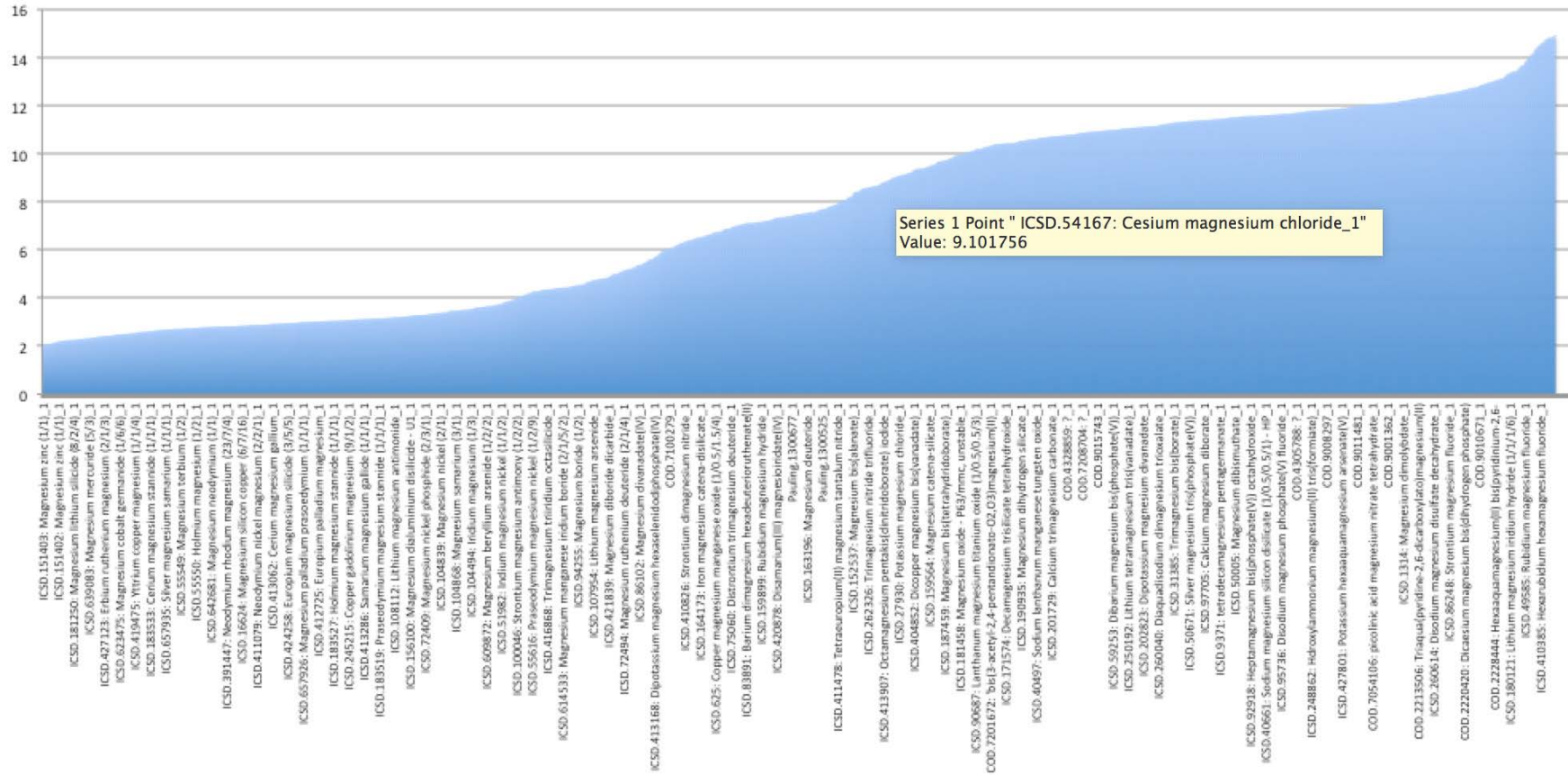
MedeaA: structure list editor
File Add structure(s) Display Properties QT: QSAR Toolbox
SQLite structure list file (8258560 bytes): C:/Users/clive/Desktop/AnnotatedWithMagnesiumEnergy1.sll
Containing 1442 structure(s)
View structures from: 1 to: 1442 Apply

Order	Name	Structural Formula	# atoms	# configurations	Symmetry	Cell parameters	MagnesiumExtractionE
1	ICSD.262083: Magnesium bis(tetrahydridoborate) - HP phase_1	Mg2B4H16	22	1	P1	5.4361 5.4361 6.1468 90 90 90	9.07670799999999964
2	COD.9007818_1	Mg2Cl4O20	26	1	P1	7.471 7.471 9.98 90 90 90	11.6783329999999995
3	COD.2013721: hexaaquamagnesium(II) benzene-1,2,4,5-tetracarbo	MgC10O14H16	41	1	P1	6.447 9.942 6.455 90 115.148 90	13.02423199999999984
4	ICSD.417035: Tetragadolinium trimagnesium dicobalt_1	Gd4Co2Mg3	9	1	P1	7.54 3.741 8.225 90 109.65 90	2.65714400000000024
5	ICSD.416490: Neodymium cobalt magnesium (4/2/3)_1	Nd4Co2Mg3	9	1	P1	7.6542 3.8053 8.3247 90 109.79 90	2.62063300000000051
6	ICSD.416491: Samarium cobalt magnesium (4/2/3)_1	Sm4Co2Mg3	9	1	P1	7.6012 3.7711 8.2684 90 109.68 90	2.63540800000000053
7	ICSD.417036: Tetraterbium trimagnesium dicobalt_1	Tb4Co2Mg3	9	1	P1	7.504 3.7286 8.195 90 109.48 90	2.66075699999999967
8	ICSD.190935: Magnesium dihydrogen silicate_1	MgSiO4H2	8	1	P1	4.756 4.266 2.844 90 90 92.99	10.5414870000000004
9	ICSD.27533: Magnesium silicate - model I_1	Mg8Si4O16	28	1	P1	10.11 5.77 4.7 90 90 90	10.0804090000000003
10	ICSD.419312: Dibarium magnesium digermanate_1	Ba4Mg2Ge4O14	24	1	P1	8.3667 8.3667 5.542 90 90 90	11.347799999999972
11	ICSD.81117: Dibarium magnesium disilicate_1	Ba4Mg2Si4O14	24	1	P1	8.2036 8.2036 5.4058 90 90 90	11.3375369999999998
12	ICSD.50065: Dicalcium magnesium disilicate_1	Ca4Mg2Si4O14	24	1	P1	7.8338 7.8338 5.0082 90 90 90	11.5118850000000007
13	ICSD.261224: Dieuropium magnesium disilicate_1	Eu4Mg2Si4O14	24	1	P1	8.0138 8.0138 5.1711 90 90 90	11.572429
14	ICSD.420522: Distrontium magnesium digermanate_1	Sr4Mg2Ge4O14	24	1	P1	8.1725 8.1725 5.315 90 90 90	11.39148799999999981
15	ICSD.261226: Distrontium magnesium disilicate_1	Sr4Mg2Si4O14	24	1	P1	8.0107 8.0107 5.1636 90 90 90	11.4671810000000011
16	ICSD.51245: Magnesium chloride_1	MgCl2	3	1	P1	4.06 4.06 4.188 90 90 90	8.64410099999999991
17	ICSD.416341: Magnesium boride carbide (2/24/1)_1	Mg4B48C2	54	1	P1	8.9391 8.9391 5.0745 90 90 90	4.56146799999999908
18	ICSD.165651: Magnesium bis(tetrahydridoborate)_1	Mg4B8H32	44	1	P1	8.18 8.18 9.965 90 90 90	10.2877060000000014
19	ICSD.249592: Strontium magnesium indide (1/1/3)_1	Sr2Mg2In6	10	1	P1	4.6895 4.6895 12.629 90 90 90	2.5876070000000002
20	COD.4328859: ?_1	Nd26Mg4Si8B16O86	140	1	P1	9.1691 15.8763 11.78 90 106.12 90	10.7808909999999883
21	ICSD.30654: Trimagnesium manganese dimanganese(III) diborate	Mn6Mg6B4O20	36	1	P1	5.36 5.98 12.73 90 120.57 90	6.770405999999999799
22	COD.4118939: ?_1	Na6Mg2P2C2O14	26	1	P1	8.82663 6.61646 5.15605 90 89.6919 90	10.4757979999999998
23	ICSD.67816: Potassium manganese tetracopper trivanadium oxide	K2V6Cu8Mg2O26	44	1	P1	10.7144 6.0282 8.3365 90 98.075 90	9.49817600000000008
24	ICSD.94669: Strontium magnesium fluoride - II_1	Sr12Mg12F48	72	1	P1	7.8249 7.493 16.9248 90 90 105.041	14.49419699999999986
25	ICSD.78532: Sodium lanthanum magnesium tellurium(VI) oxide_1	Na2La2Mg2Te2O12	20	1	P1	5.5526 5.5349 7.9126 90 90.22 90	10.4375139999999993
26	ICSD.40497: Sodium lanthanum manganese tungsten oxide_1	Na2La2W2Mg2O12	20	1	P1	5.5239 5.5253 7.8939 90 90.16 90	10.61518799999999989
27	ICSD.150576: Magnesium zinc (1/2) - eta'_1	Mg2Zn4	6	1	P1	4.97 5.54 4.97 90 120 90	2.62803700000000008
28	COD.9010402_1	Mg6Si6O18	30	1	P1	7.026 6.228 4.262 90 95.85 90	7.38787700000000031
29	COD.9010401_1	Mg8Si8O24	40	1	P1	9.477 6.205 4.256 90 98.75 90	7.21475100000000068
30	ICSD.187151: Magnesium silber antimonide_1	As16Mg16S16	48	1	P1	0.1761 0.1761 12.606 90 90 90	2.22722000000000051

Close



Énergies de Liaison du Magnésium

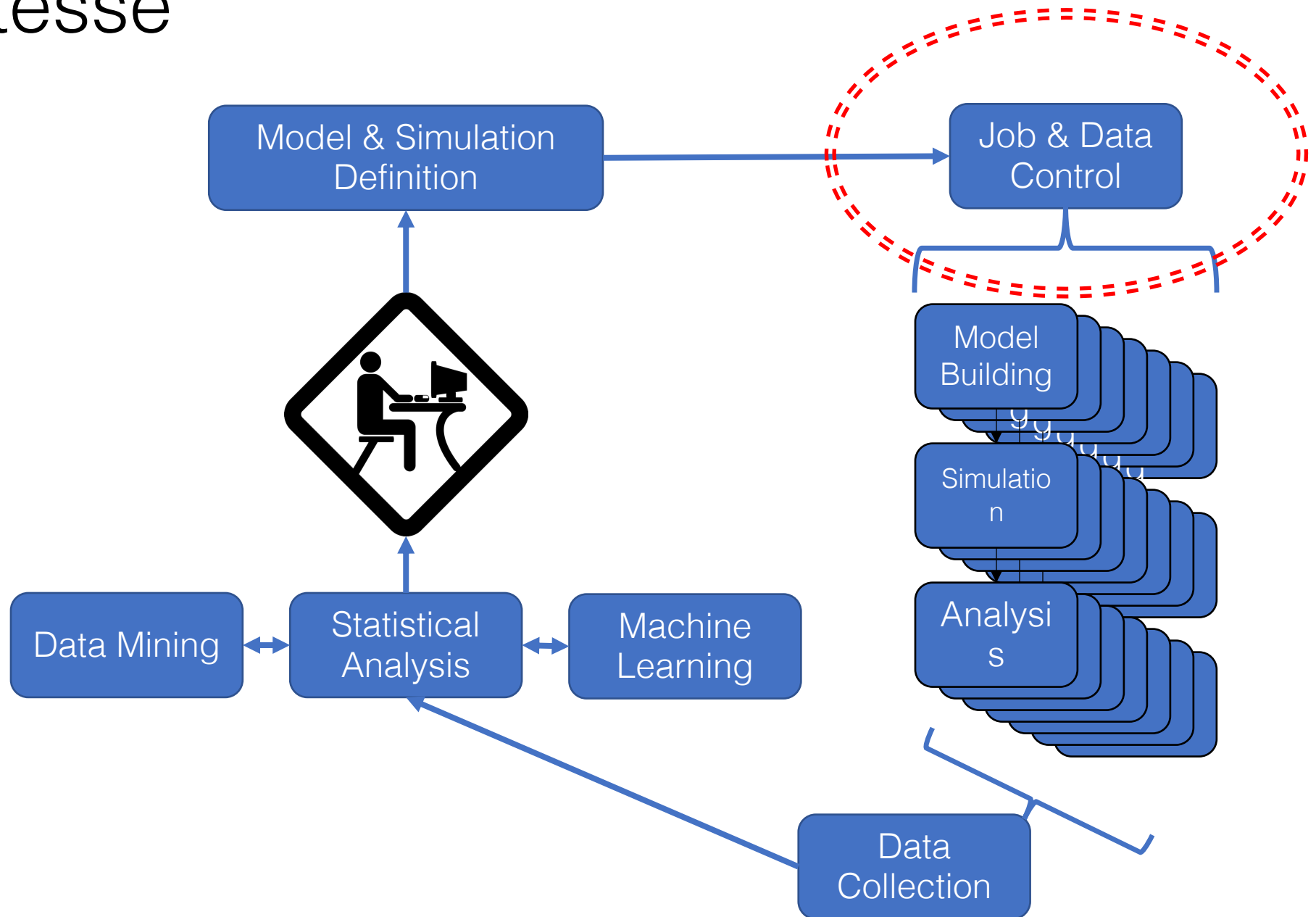


- Ranking of the magnesium removal energies



Infrastructure et Calculs Haut Débit dans *MedeA* : Atouts, Robustesse et Versatilité

Robustesse



Mise en Œuvre du Calcul Haut Débit dans *MedeA*

The image displays the MedeA software interface for configuring a high-throughput calculation. The main window is titled "Materials Design Flowchart" and shows a "Start" button. A dialog box titled "Edit ForEach Structure stage 1" is open, showing the "Flowchart" tab. The "From a previous stage" radio button is selected. The "Structure list file" field is empty. A warning message states: "Warning: Preparing a flowchart with VASP requires an active window system. After setting up the VASP calculation parameters for this system, they are indentially used for all structures in the list afterwards." The "Advanced settings" checkbox is unchecked. The "Run the different loop iterations simultaneously" checkbox is checked, and the "Maximum number of jobs to submit simultaneously" is set to 20. The "Catch and ignore errors in the iterations" checkbox is unchecked. The "OK" and "Cancel" buttons are visible at the bottom of the dialog. A "Submit Run job" dialog box is also open, showing the "Queue" set to "ContractMontrouge", "Number of processors" set to 16, and "Priority" set to 5. The "Run" and "Cancel" buttons are visible at the bottom of this dialog. Green arrows and dashed circles highlight the "Run the different loop iterations simultaneously" checkbox, the "Maximum number of jobs to submit simultaneously" input field, and the "OK" button in the "Submit Run job" dialog.

- Value: Highly efficient screening of large number of compounds

Mise en Œuvre du Calcul Haut Débit dans *MedeA*

Run the different loop iterations simultaneously Maximum number of jobs to submit simultaneously X



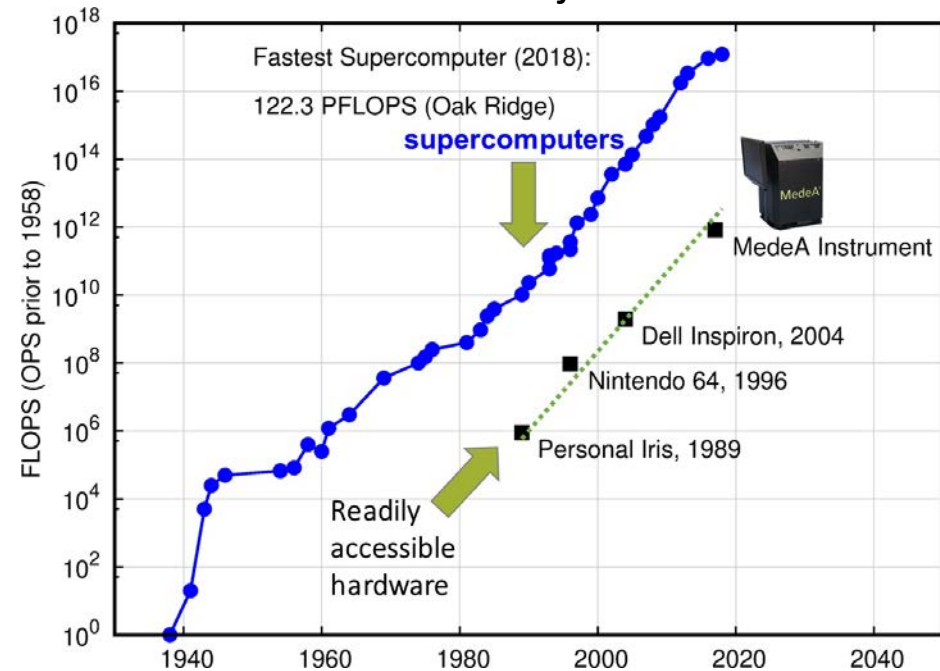
4 jobs × 1 core



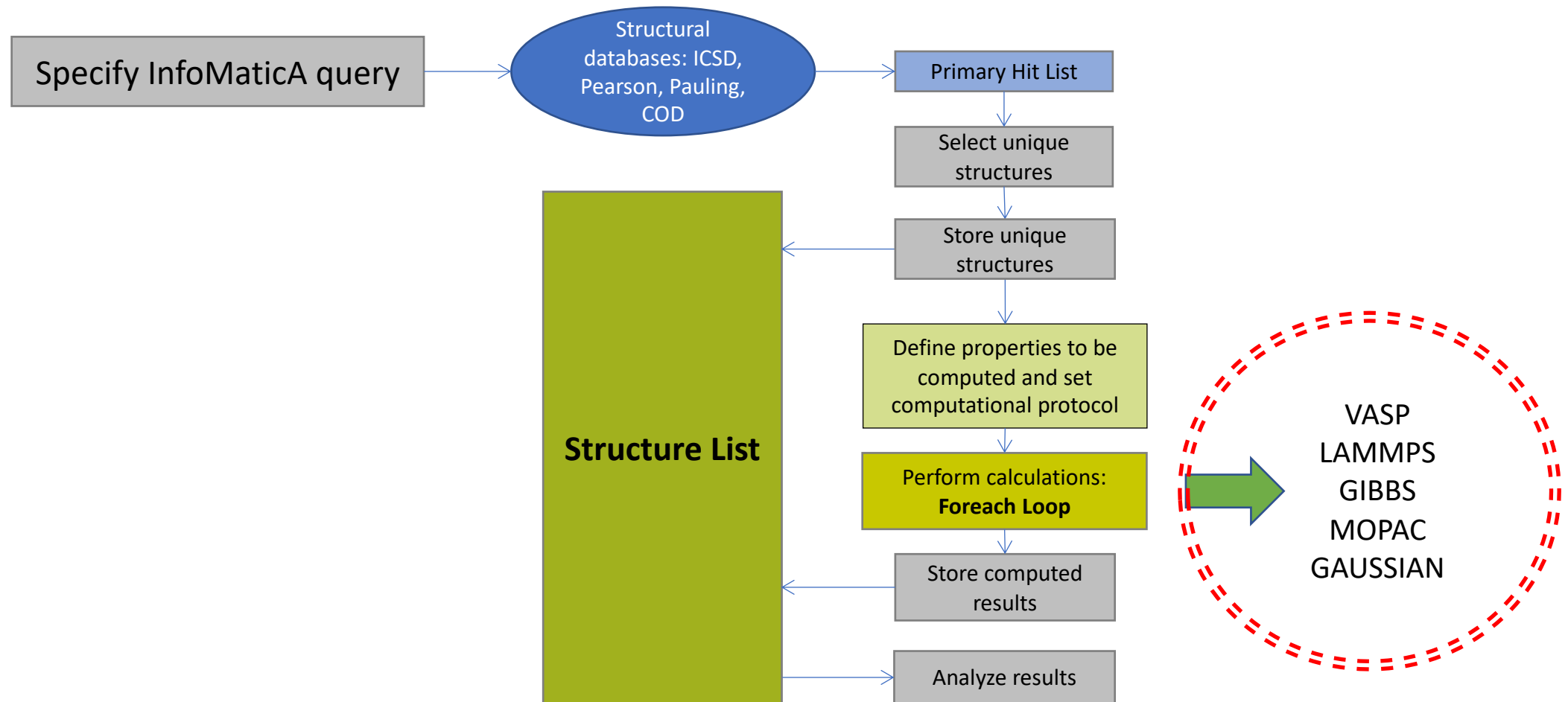
10 jobs × 8-16 cores



100 jobs × 32 cores

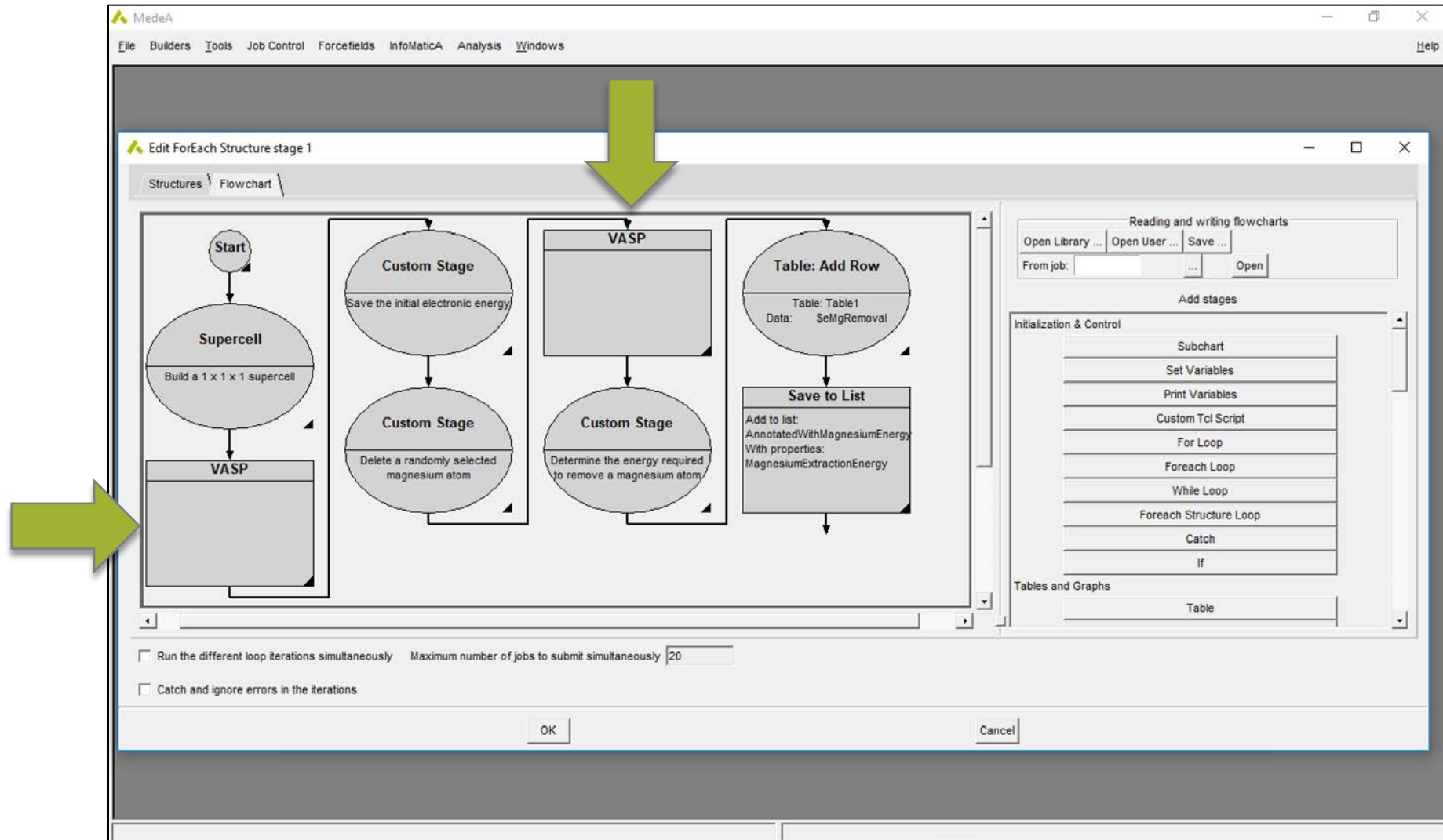


Versatilité



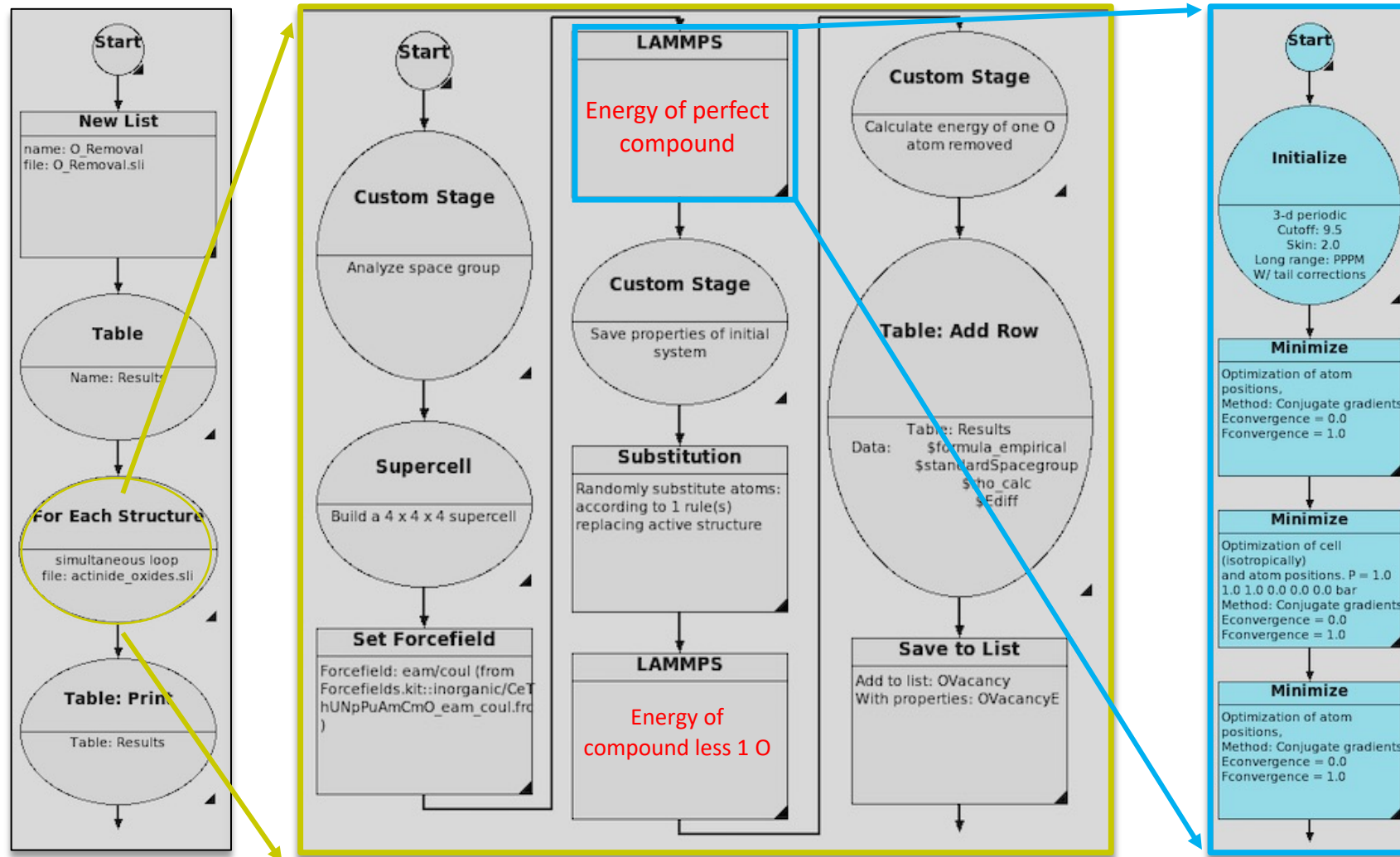


Calculs Haut Débit : Robustesse et Versatilité - VASP





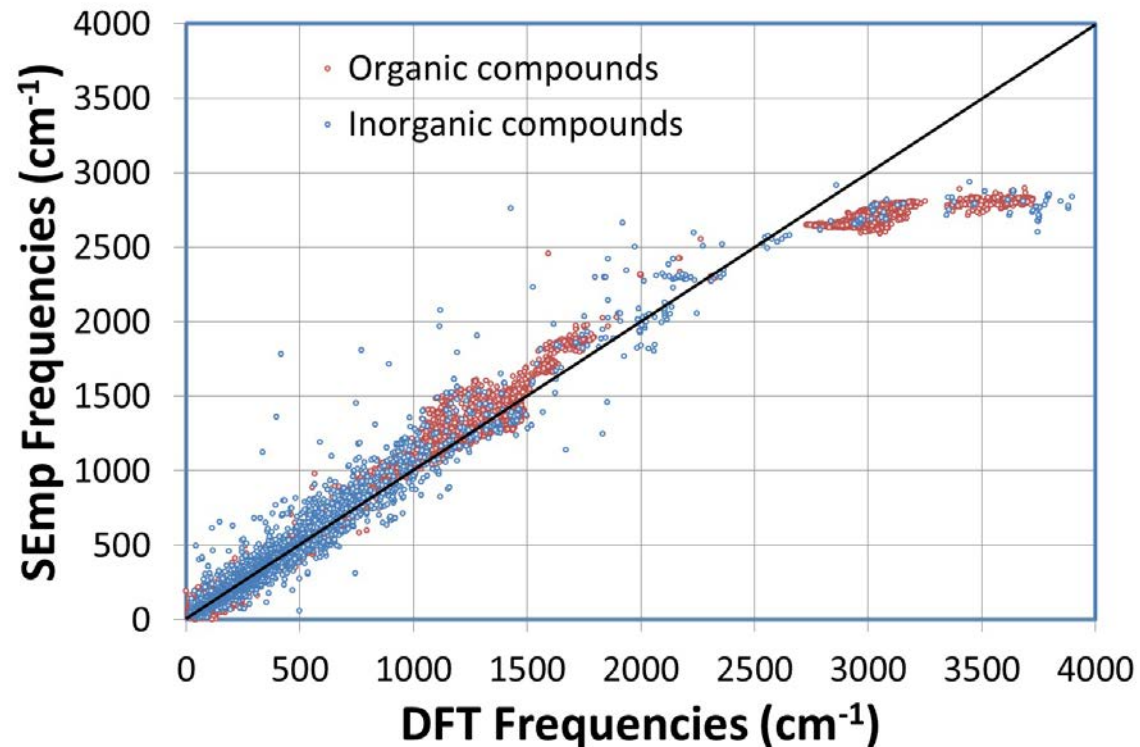
Calculs Haut Débit : Robustesse et Versatilité - LAMMPS





Calculs Haut Débit: Robustesse et Versatilité – GAUSSIAN et MOPAC

- ▶ Comparison between the vibrational frequencies computed with semi-empirical and DFT methods for organic and inorganic molecules: 1395 molecules, ~42,000 frequencies

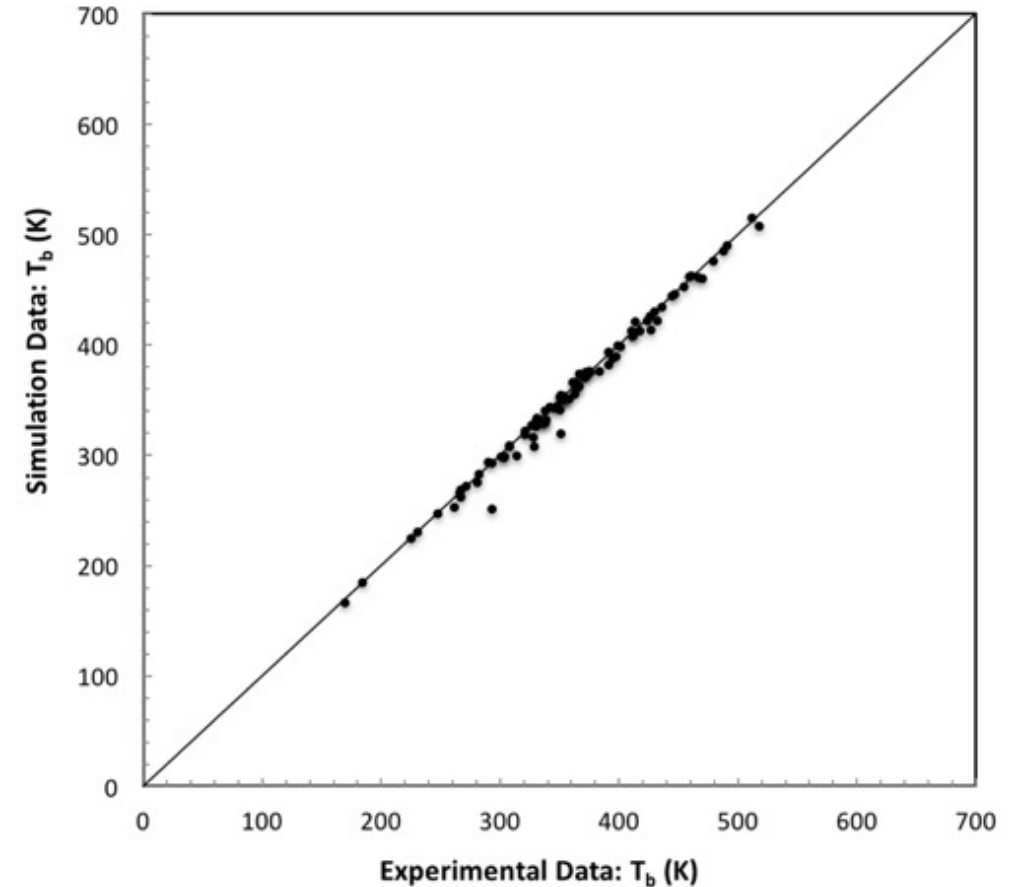
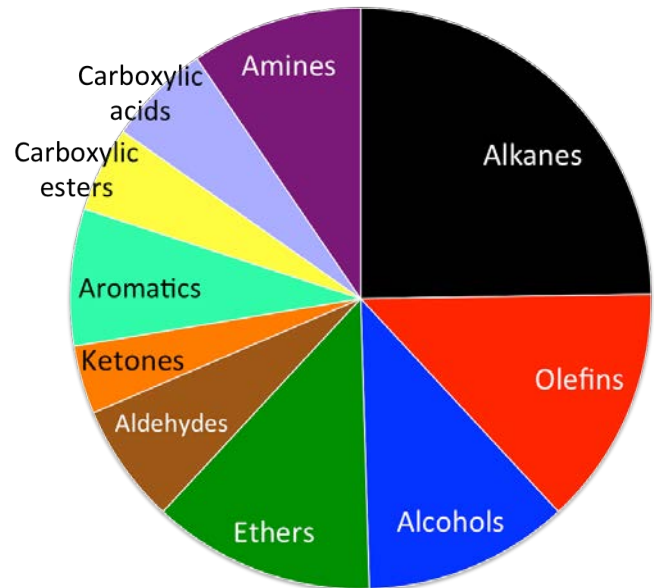


Rozanska *et al.* *J. Chem. Eng. Data* **2014**, *59*, 3136-3143 & *Oil Gas Sci. Tech.* **2015**, *70*, 405-417



Calculs Haut Débit : Robustesse et Versatilité – Monte Carlo GIBBS

- ▶ Sample shown in the plot: ~100 compounds
- ▶ AAD of the T_b calculated by GEMC simulation from the DIPPR* data, is 1.4%
- ▶ More than half of the compounds have an Absolute Deviation (AD) of the T_b below 1.0%

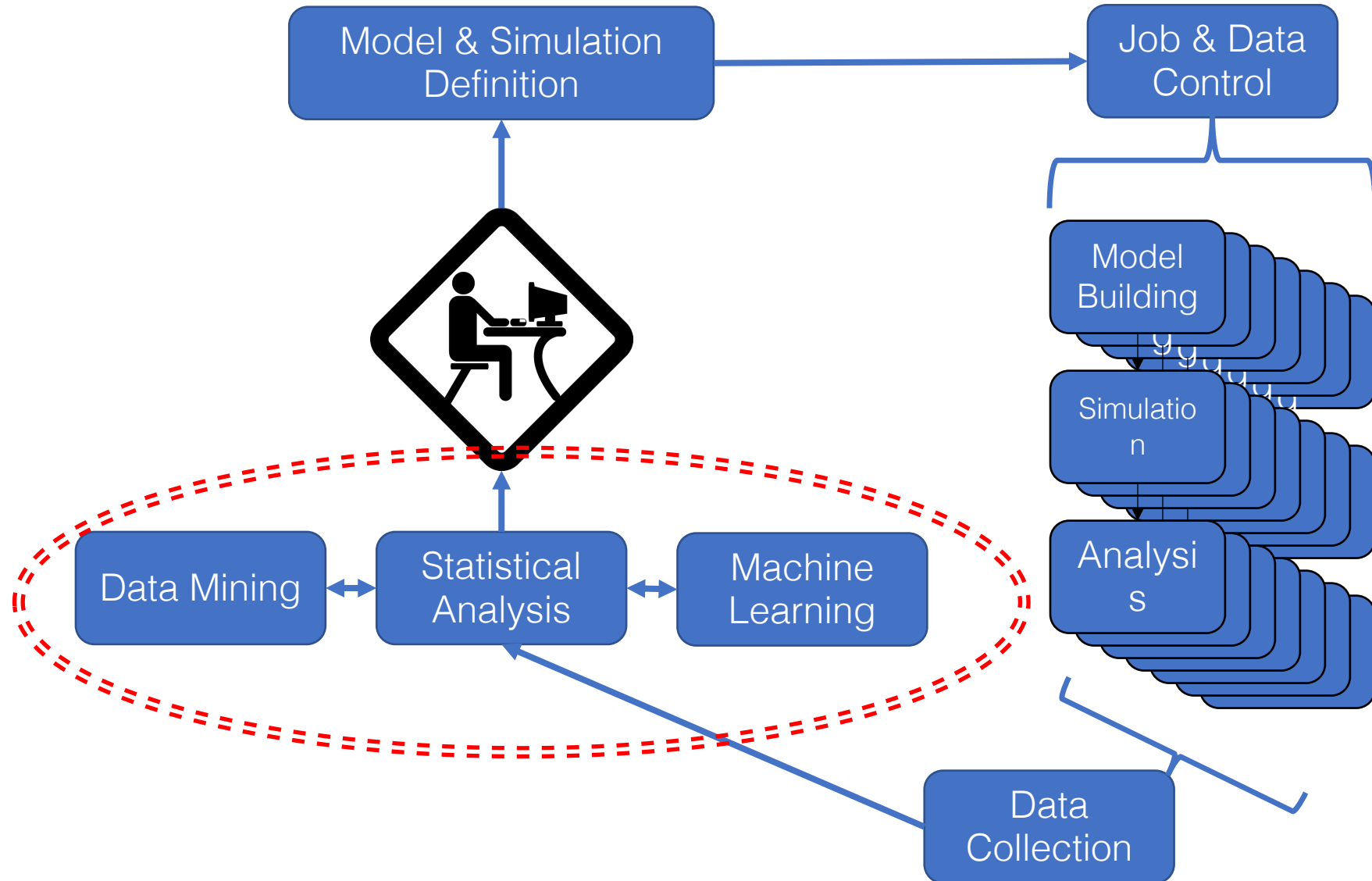


MedeA-GIBBS simulations (AUA & TraPPE-UA FF)



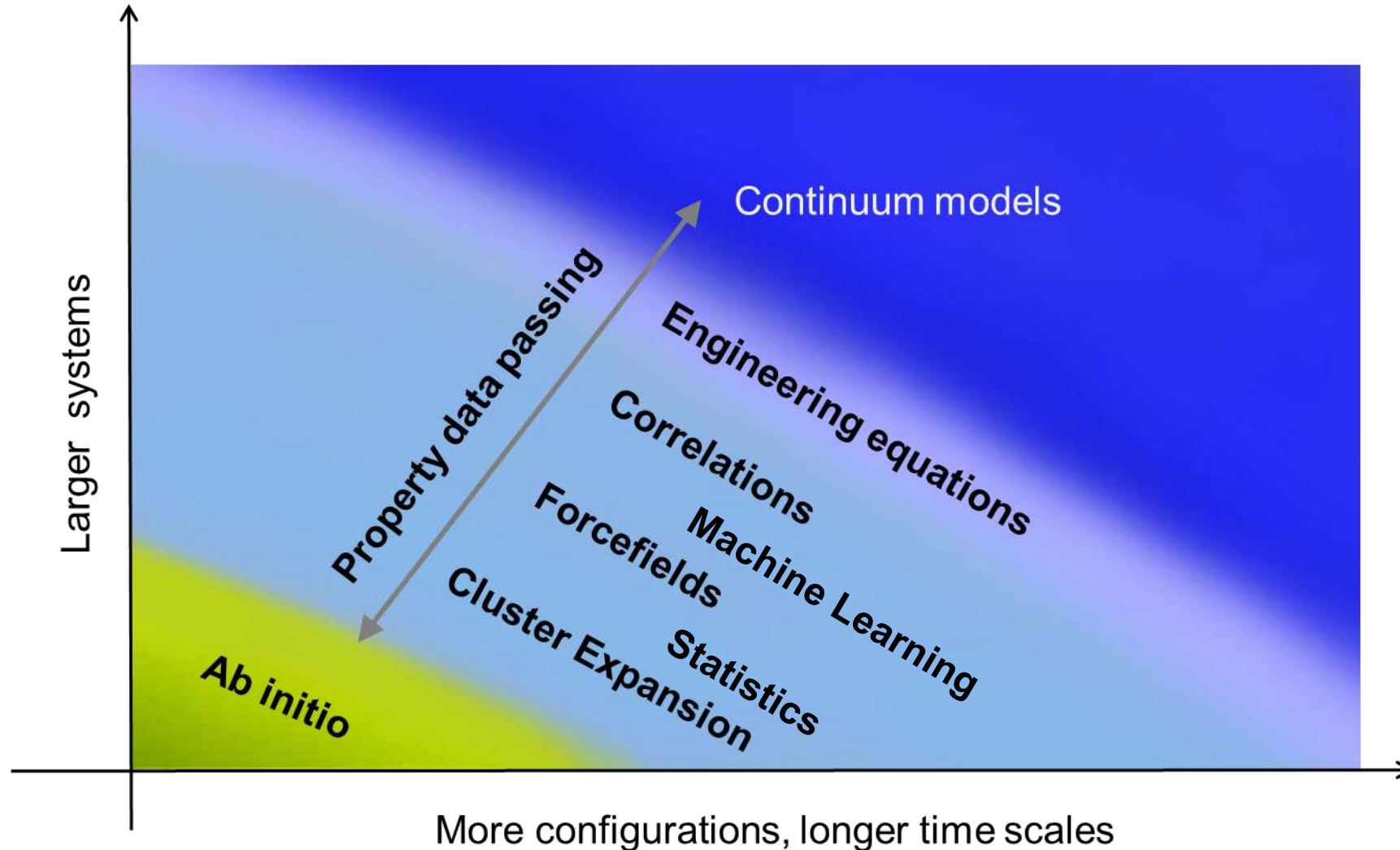
Exploitation Subséquente du Calcul
Haut Débit dans *MedeA*:
Corrélation, Champs de Forces et
Auto-Apprentissage

Analyse et Exploitation des Données





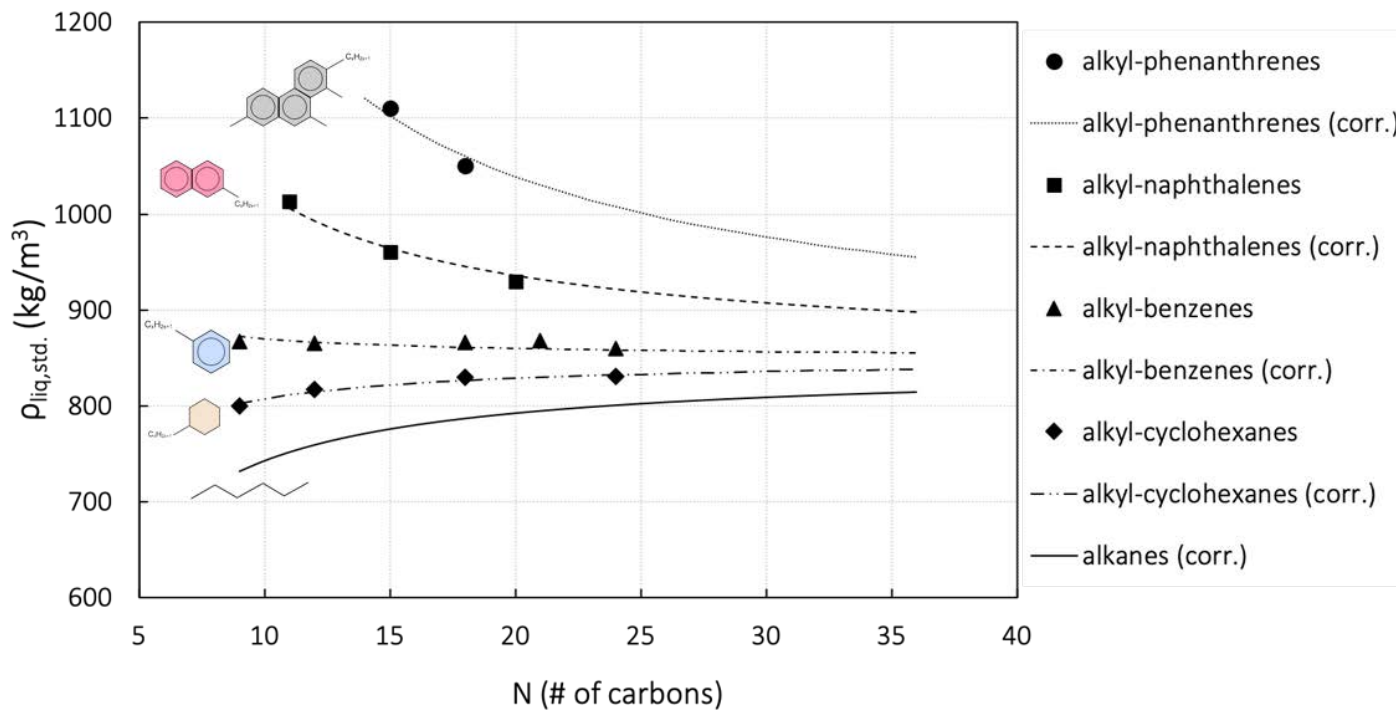
Liaisons entre propriétés et modèles par changement d'échelles de temps et de taille



Modèles de Corrélation

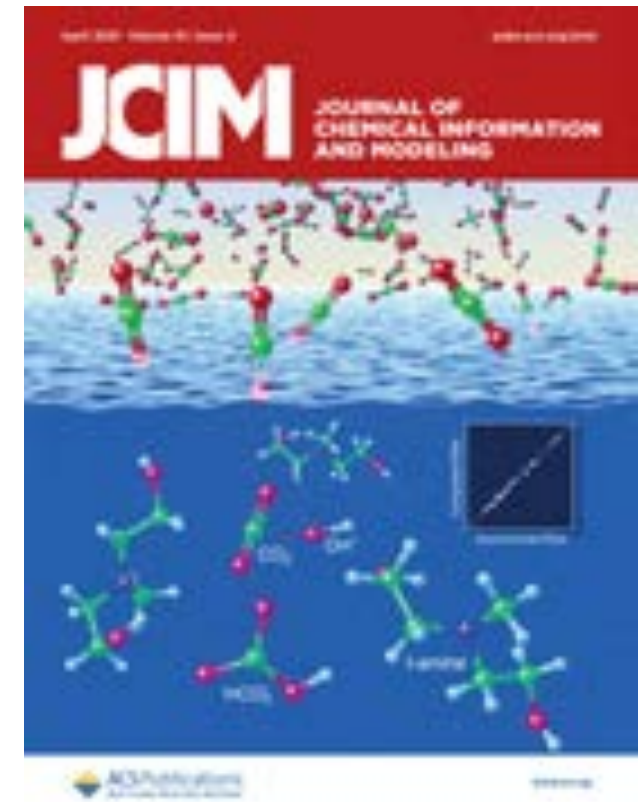
Use correlations to predict properties for other members of a chemical family

Heavy Crude Oil Components
Liquid Density Prediction



Ungerer et al. *Energy Fuels* **2019**, *33*, 2967

CO₂ Absorption Kinetics



Rozanska et al. *J. Comput. Chem. Inf. Model.* **2021**, *61*, 1814

Éditeur de Liste de Structures : Propriétés et Descripteurs

- *MedeA* offers a consistent basis for the construction of descriptors and correlations

The image shows two overlapping windows from the MedeA software. The left window is the 'MedeA: structure list editor' and the right window is the 'MedeA: structure list descriptors' dialog.

MedeA: structure list editor

File Add structure(s) Display **Properties**

SQLite structure list file (547840 byte)
Containing 500 structure(s)

New property
Descriptors
Delete

View structures from: 1 to: 200 Apply

Order	Name
18	ICSD.188829: Lithium beryllium (1/1)
41	ICSD.246613: Lithium palladium hydride (1/1/1)
3	ICSD.187135: Lithium iron phosphide
2	ICSD.187132: Lithium iron arsenide
154	Pearson.1702887
58	Pearson.1713560
40	ICSD.616780: Bismuth lithium (1/1)
66	COD.9016055

MedeA: structure list descriptors

Atomic radii in voids and coordination Covalent Ionic

Load catalog Save catalog Clear

Descriptors catalog

Descriptor	Assigned property
sumhvyatgroup	sumhvyatgroup
ngnc0	ngnc0
ngnc1	ngnc1

Descriptor definition

Name: sumhvyatgroup

Existing descriptors Structure properties Atomic properties Ligand properties Voids properties

Generic functions Atom functions Ligand functions

Atomic number Coordination class

Expression: @nbr1+@nc0+@nc1+@nc10+@nc11+@nc12+@nc13+@nc14+@nc15+@nc2+@nc3+@nc4+@nc5+@nc6+@nc7+@nc8+@nc9+@nc16+@nc17+@nc18+@nc19+@nc20+@nc21+@nc22+@nc23+@nc24+@nc25+@nc26+@nc27+@nc28+@nc29+@nc30+@nc31+@nc32+@nc33+@nc34+@nc35+@nc36+@nc37+@nc38+@nc39+@nc40+@nc41+@nc42+@nc43+@nc44+@nc45+@nc46+@nc47+@nc48+@nc49+@nc50+@nc51+@nc52+@nc53+@nc54+@nc55+@nc56+@nc57+@nc58+@nc59+@nc60+@nc61+@nc62+@nc63+@nc64+@nc65+@nc66+@nc67+@nc68+@nc69+@nc70+@nc71+@nc72+@nc73+@nc74+@nc75+@nc76+@nc77+@nc78+@nc79+@nc80+@nc81+@nc82+@nc83+@nc84+@nc85+@nc86+@nc87+@nc88+@nc89+@nc90+@nc91+@nc92+@nc93+@nc94+@nc95+@nc96+@nc97+@nc98+@nc99

Description:

OK Cancel

Close Help

Descriptors catalog

cage_diameter (Ang)
cross_diameter (Ang)
delta_cage_diameter (Ang)
delta_cross_diameter (Ang)
delta_void_volume (Ang^3)
void_class
void_volume (Ang^3)



Optimisation de Paramètres de Champs de Forces par Algorithme d'Évolution Génétique

MedeA Forcefield Optimizer

Fitting Data Forcefield Optimization Options Flowchart

Evolutionary Algorithm parameters

Population size

Number of generations

Multiobjective optimization

The following can be selected for multiobjective optimization. For each property such as energy or forces, linear regression is made for points located according to reference / computed values. On a perfect match the regression coefficient beta1 should be 1 (beta1 also noted in the equation 'y = a * x + b') and R should be also 1. Objective noted a means minimizing the value: abs(1.0 - a) Objective noted R means minimizing the value: abs(1.0 - R)

Total Energy

<input type="checkbox"/> RMSD	<input type="checkbox"/> a	<input type="checkbox"/> R
-------------------------------	----------------------------	----------------------------

Energy per atom

<input checked="" type="checkbox"/> RMSD	<input checked="" type="checkbox"/> a	<input checked="" type="checkbox"/> R
--	---------------------------------------	---------------------------------------

Forces

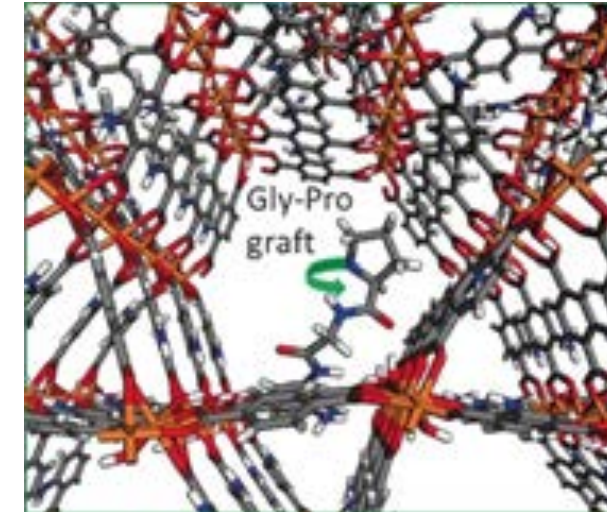
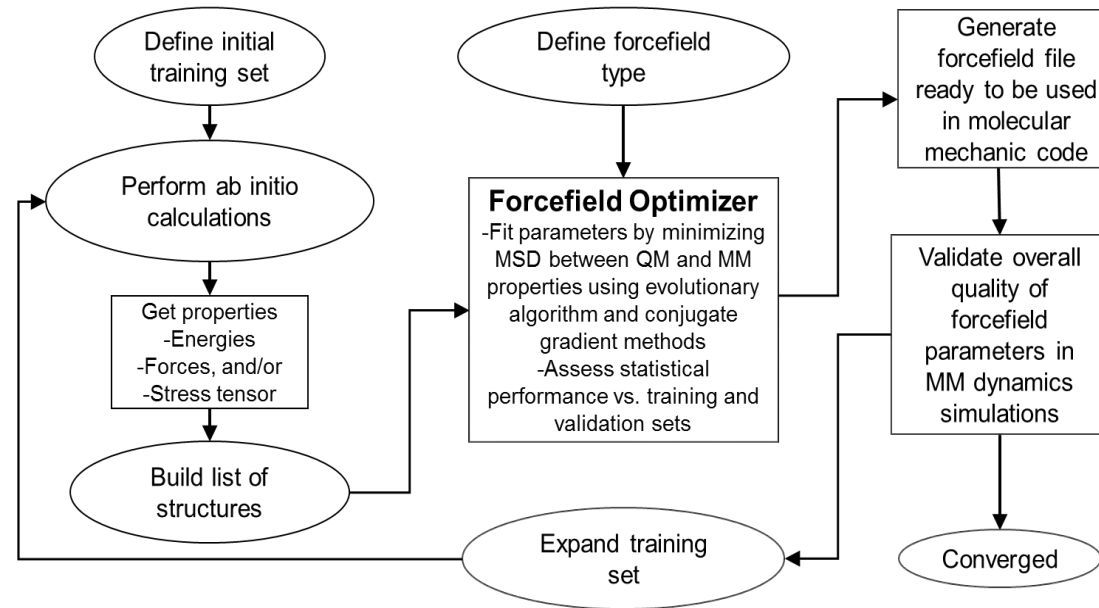
<input checked="" type="checkbox"/> RMSD	<input checked="" type="checkbox"/> a	<input type="checkbox"/> R
--	---------------------------------------	----------------------------

Stress

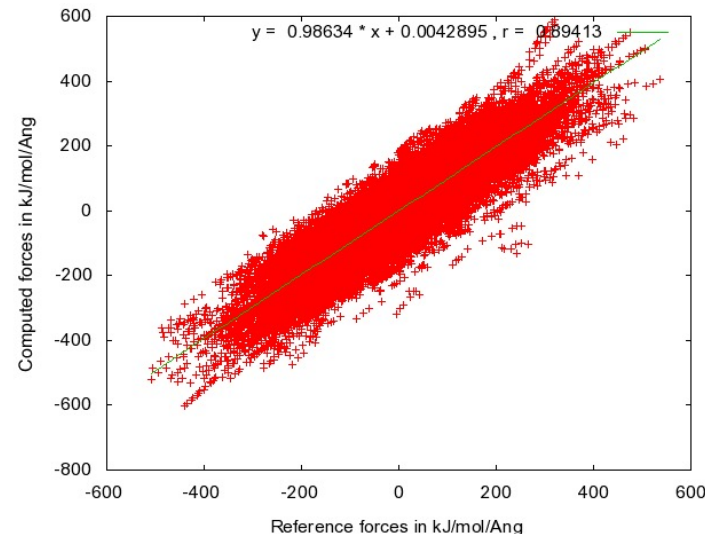
<input type="checkbox"/> RMSD	<input type="checkbox"/> a	<input type="checkbox"/> R
-------------------------------	----------------------------	----------------------------

Least Squares Fitting parameters

Maximum number of iterations	<input type="text" value="1"/>
Maximum number of function evaluations	<input type="text" value="0"/>
Finite difference step size parameter	<input type="text" value="1.0e-5"/>
Initial step size factor	<input type="text" value="100.0"/>



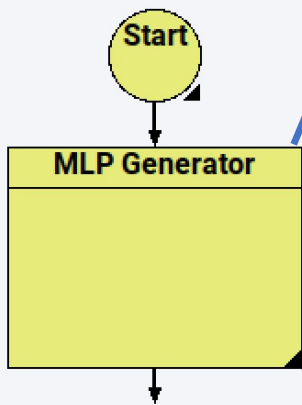
Todorova et al. *Chem. Eur. J.*, 2016, 22, 16531-16538.



Optimisation de Champs de Forces par Méthode d'Auto-Apprentissage

MedeA MLP Generator

- ▶ Uses structure list
- ▶ Provides Machine Learning Potential (MLP)



Start

MLP Generator

Edit MLP generator stage 1

Structure list:

Type of machine learning potential: SNAP

Parameters for SNAP **Advanced**

Band limit: 8

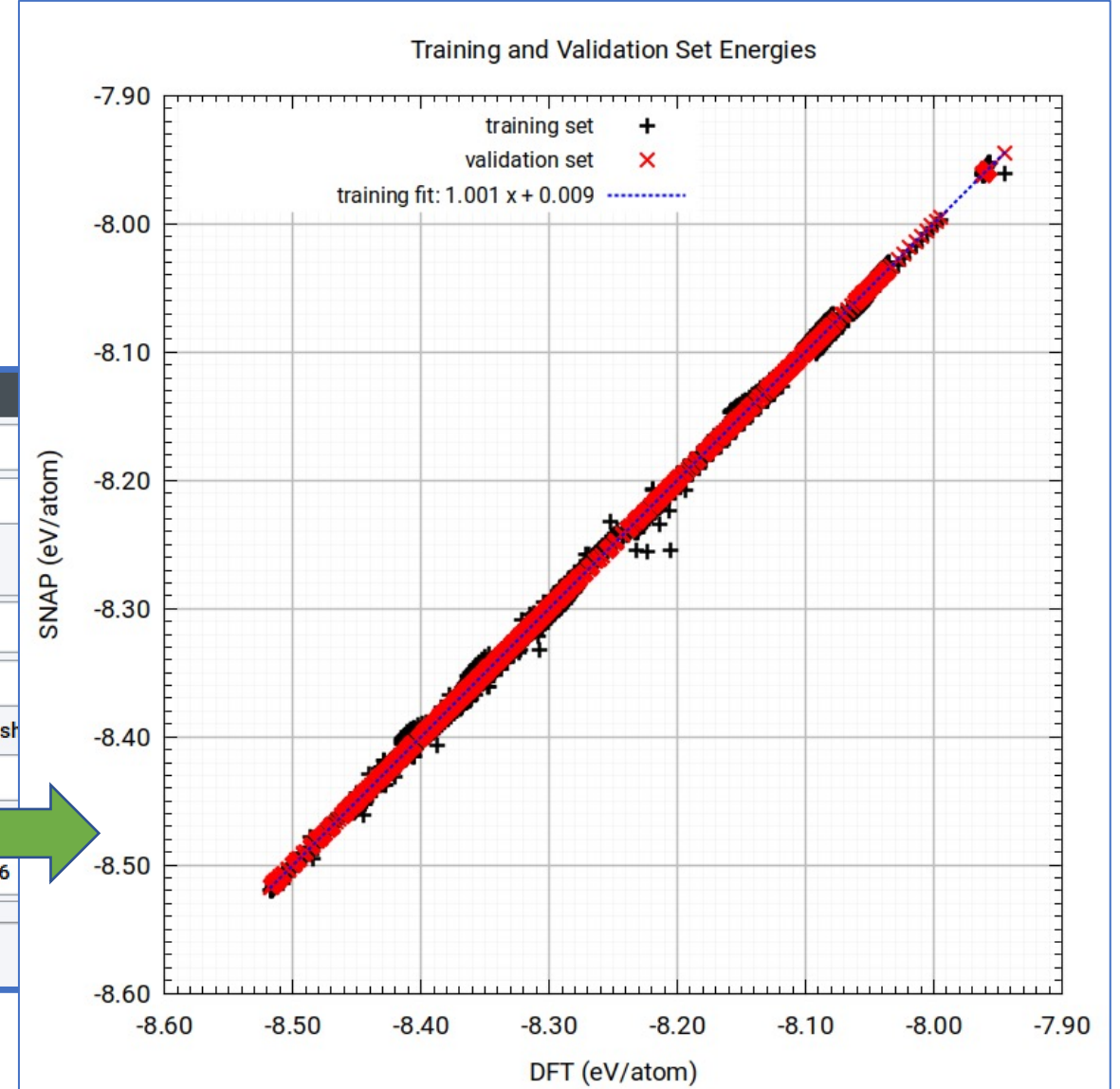
Radial cutoff: 7.01456

Element	Relative radius	Weight	Energy sh
	0.5	1.0	0.0

Fit: Energy Forces

Weights: 1.0 0.01 1.0e-06

OK Cancel





Résumé et Derniers Mots

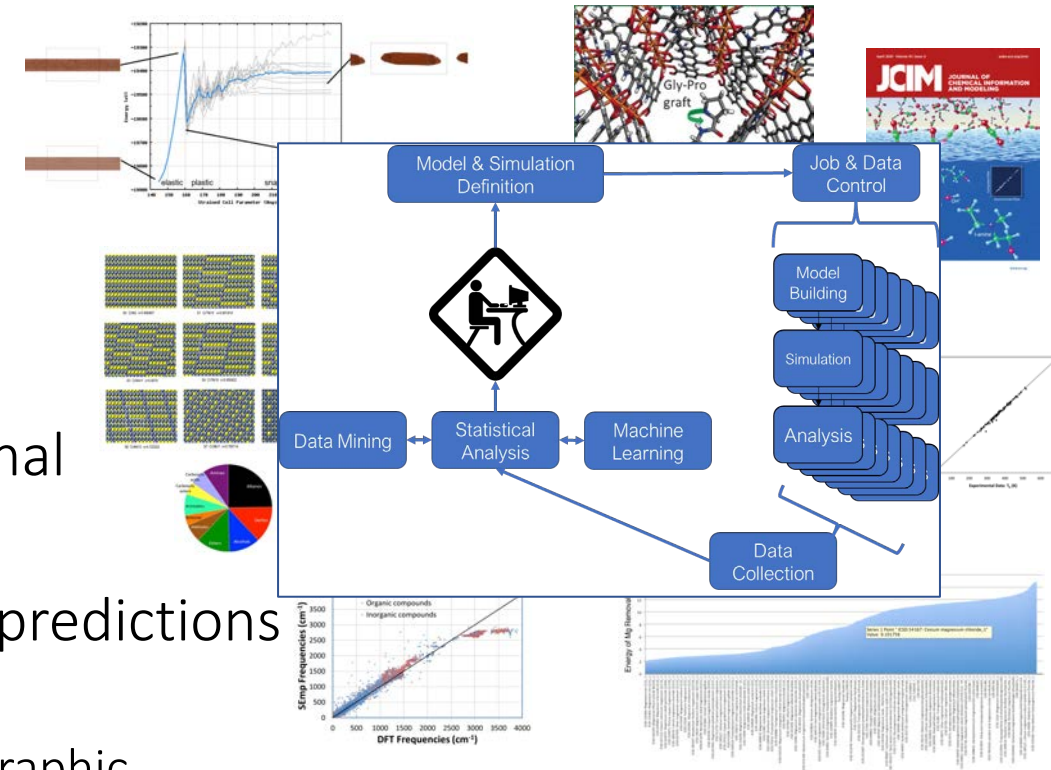


Calculs à Haut Débit dans l'Environnement Logiciel *MedeA*

- Highly efficient exploration of parameter space
 - Improving statistics
 - Scanning of variables, e.g. T , P , concentration
 - Filtering signal from noise (T_g of polymers)
- Straightforward combination of different computational approaches in a single workflow
- Comprehensive, systematic, and consistent property predictions for large sets of structures
 - Binding energy of Mg in compounds contained in crystallographic databases (ICSD, Pearson)
 - Thermodynamic properties of molecules from semi-empirical quantum mechanics calculations
 - Fluid properties

Resulting in more efficient solutions of materials problems and driving innovation

- Subsequent data exploitation and added value



High-Throughput

- ▶ MedeA modules mentioned in today's webinar

<https://www.materialsdesign.com/compute-engines>

<https://www.materialsdesign.com/analysis-tools>

[MedeA Environment](#)

[MedeA HT](#)

[MedeA VASP](#)

[MedeA LAMMPS](#)

[MedeA MOPAC](#)

[MedeA Gaussian](#)

[MedeA GIBBS](#)

[MedeA QT](#)

[MedeA Forcefield Optimizer](#)

- ▶ 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

Session de Questions et Réponses



Dr. Xavier Rozanska

Materials Design



Dr. Benoit Minisini

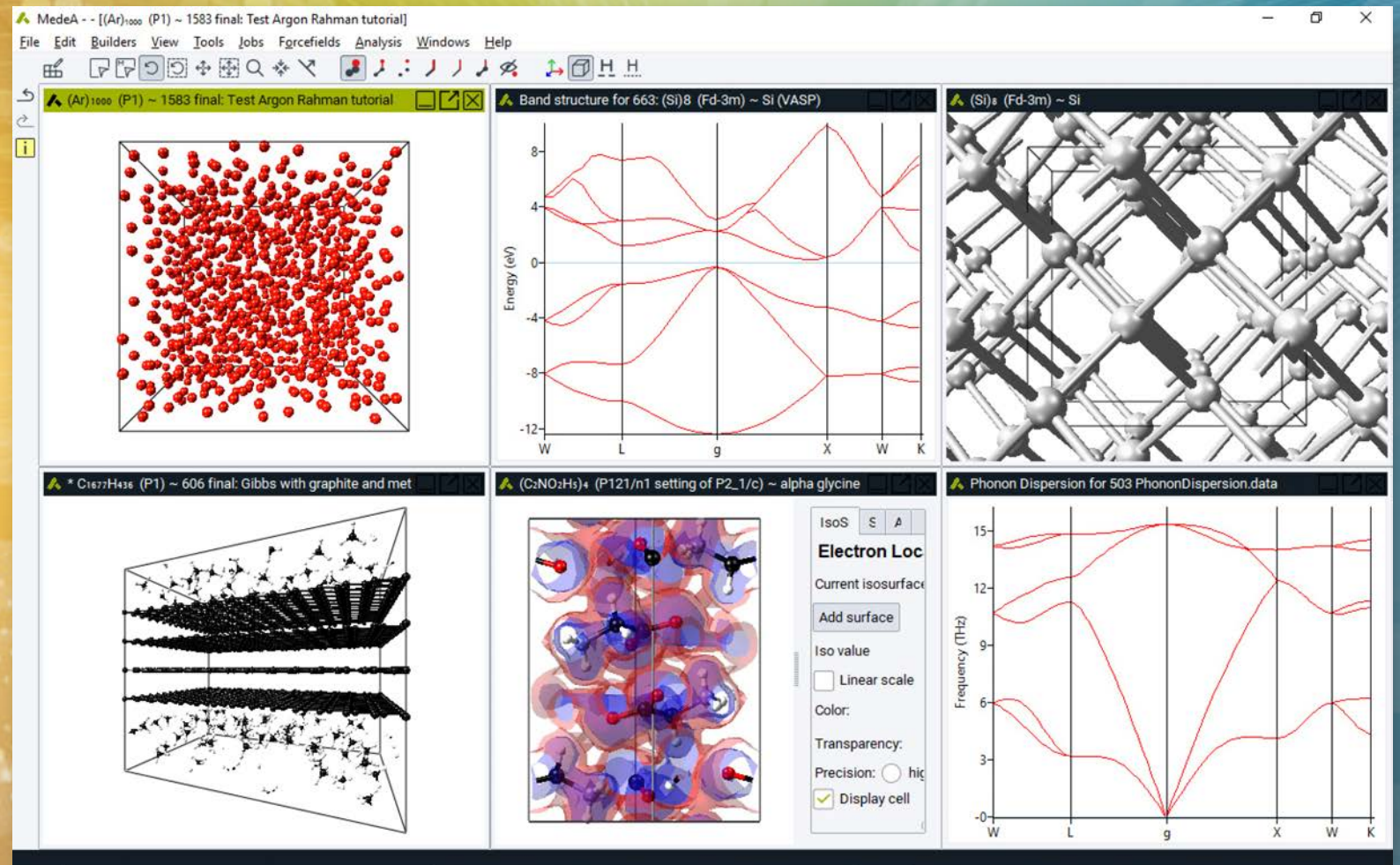
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MedeA 3.3

Software Release

July 2021

[www.materialsdesign.com/
software-releases](http://www.materialsdesign.com/software-releases)



Session de Questions et Réponses



Dr. Xavier Rozanska

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Dr. Benoit Minisini

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Pour toutes autres questions sur nos webinaires passés et futurs

Katherine Hollingsworth

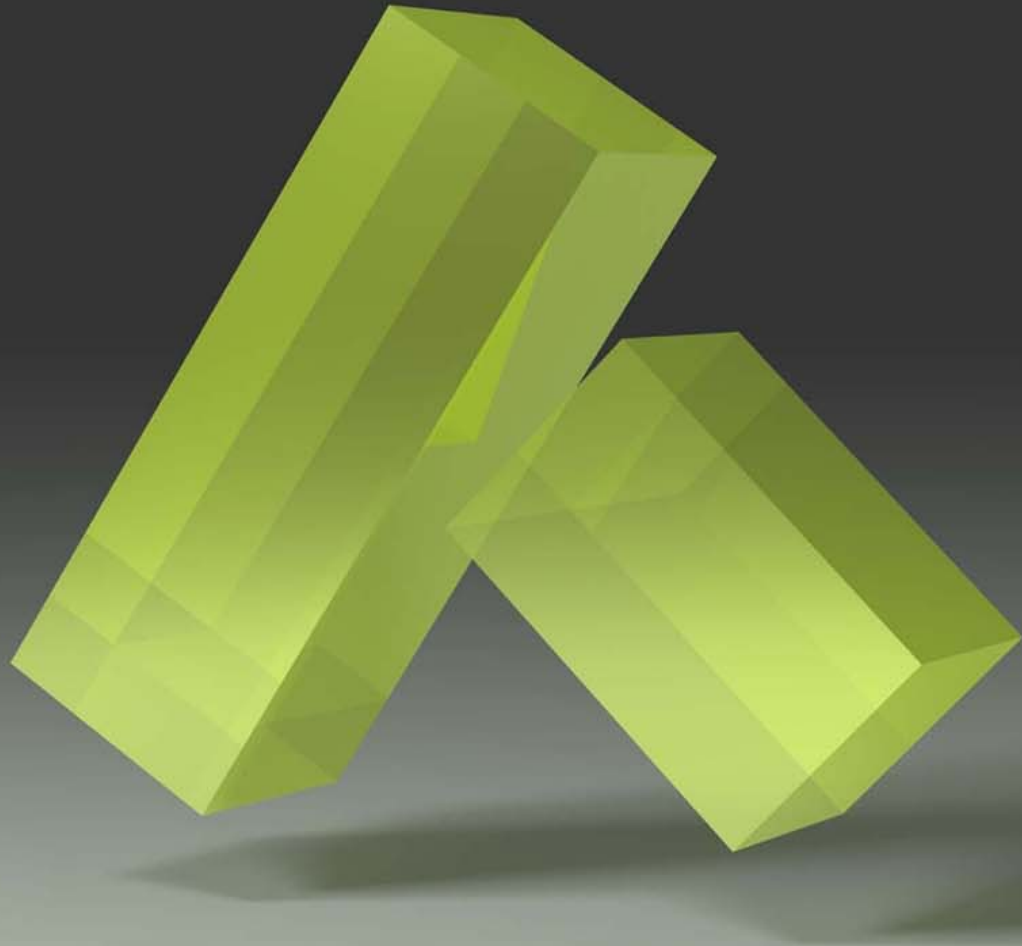
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