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

Materials Design, SARL

Juin 2021

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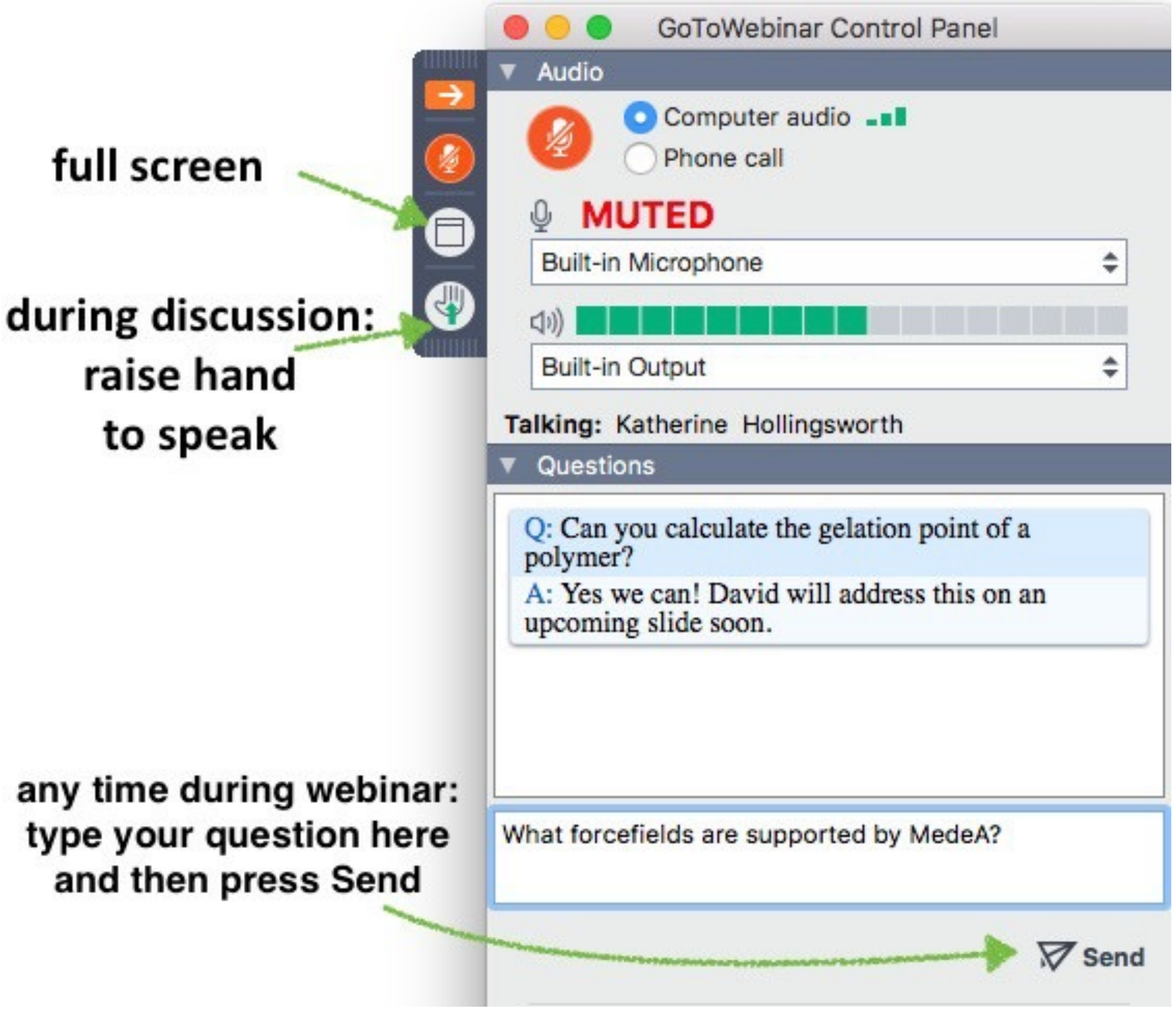

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Calculs à Haut Débit dans l'Environnement Logiciel *MedeA*

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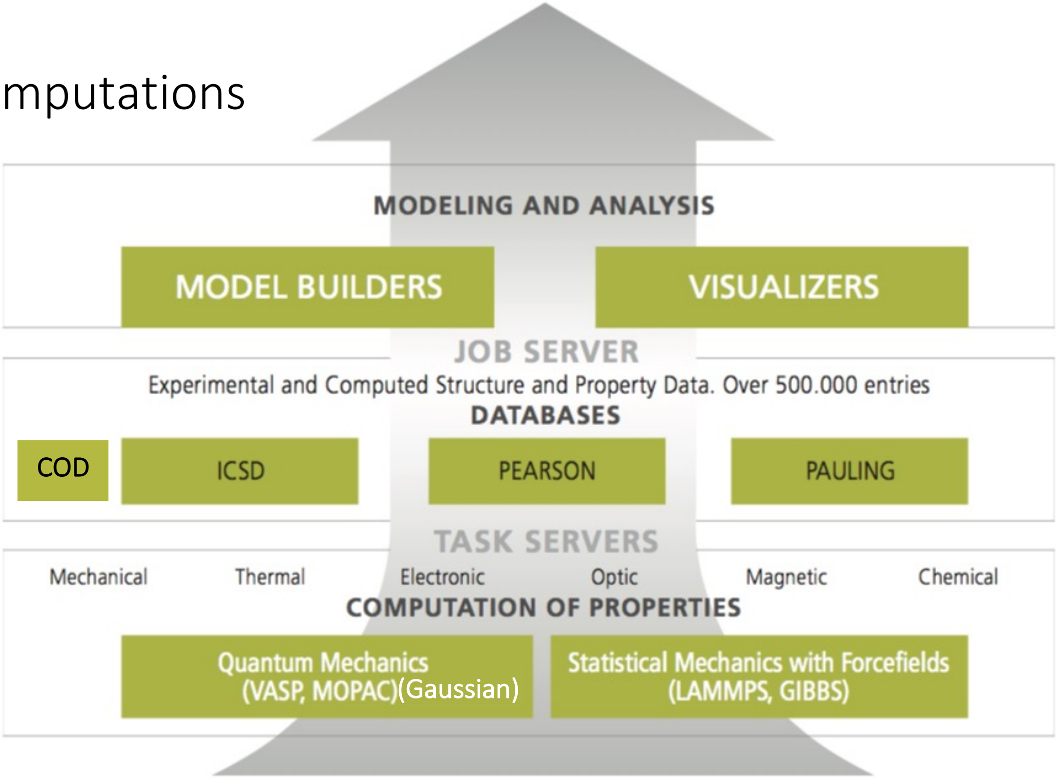
Environnement Logiciel *MedeA*

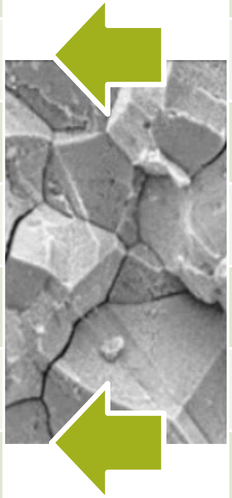
- Data central in *MedeA*
  - Integrating of experimental data with simulations
    - currently > 1 M data entries + computed data
- Fast technology development
  - High-throughput data generation by experiment and computations
  - Data storage and handling
  - Cloud computing
  - Massive parallelization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



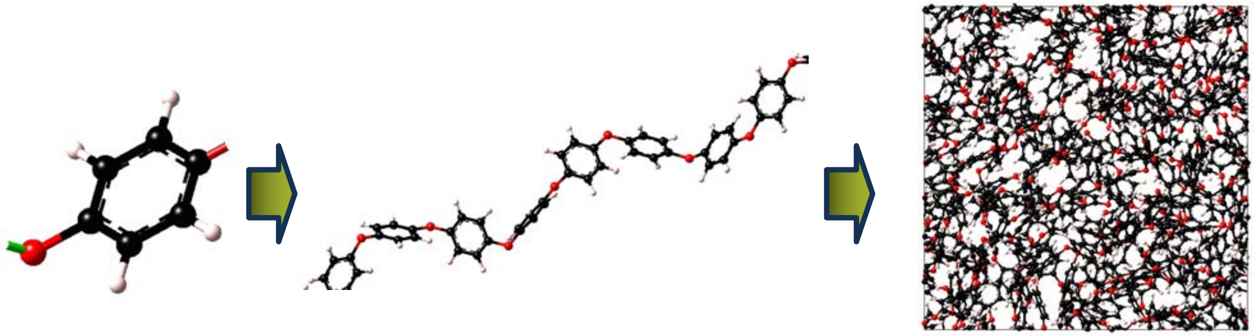
Échantillonnage et Statistique

Les propriétés des matériaux découlent de phénomènes microscopiques

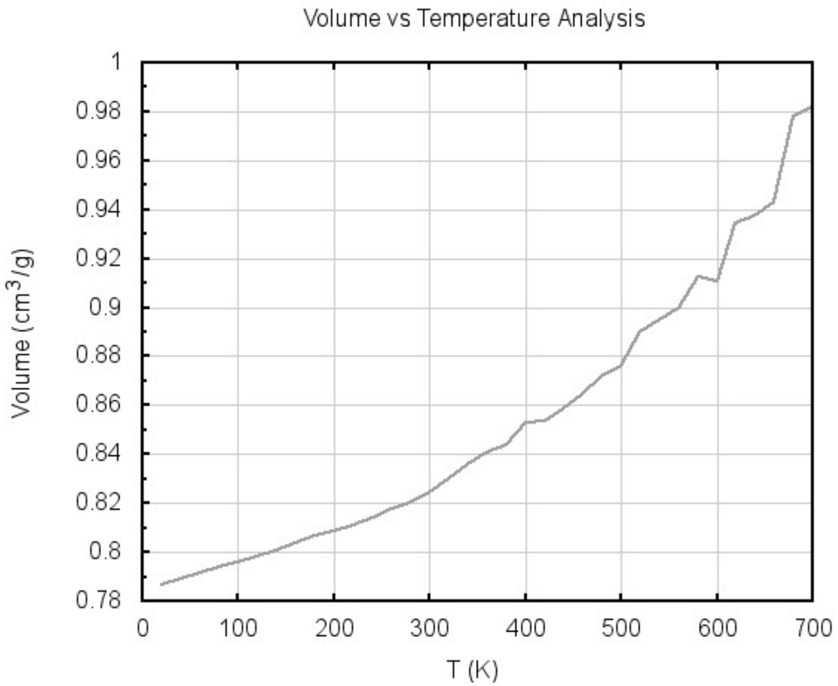
Microscopic phenomena	Atomistic descriptor
Defects, Vacancies	Formation energies
Diffusion	Activation energies (Transition states)
Interfaces/grain boundaries	Free energy, lattice mismatch, thickness
Elasticity	Elastic constants, moduli, strain analysis
Antiphase boundaries	Formation energies
Anti-sites	Formation energies
Configurational disorder	Ground states, microstructure evolution
Lattice vibrations	Phonons, Free energy as function of T
…	…



Température de Transition Vitreuse (T_g) d'un Polymère

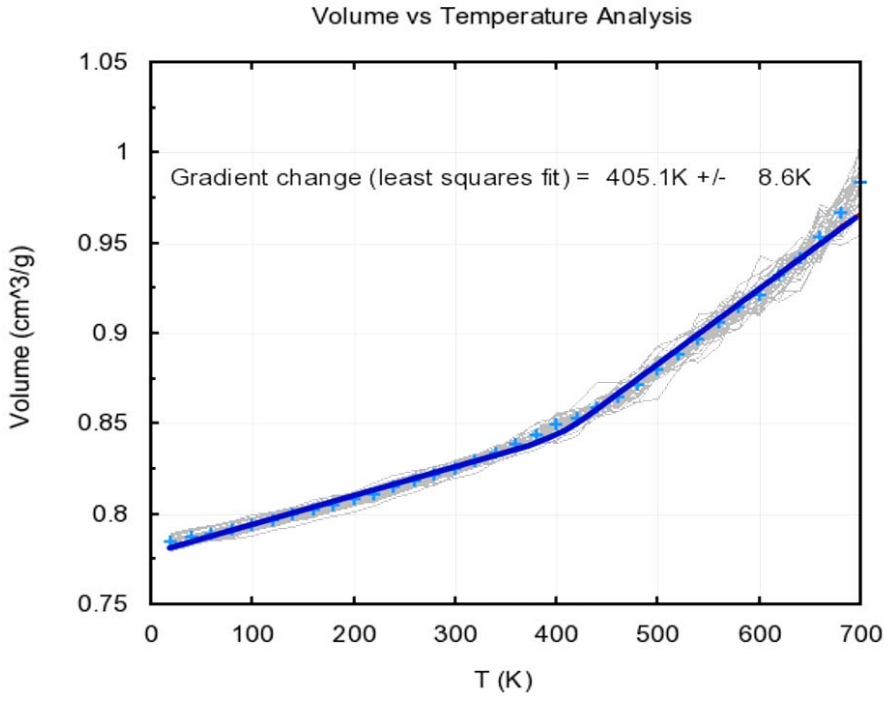


Polyphenylene ether (PPE)



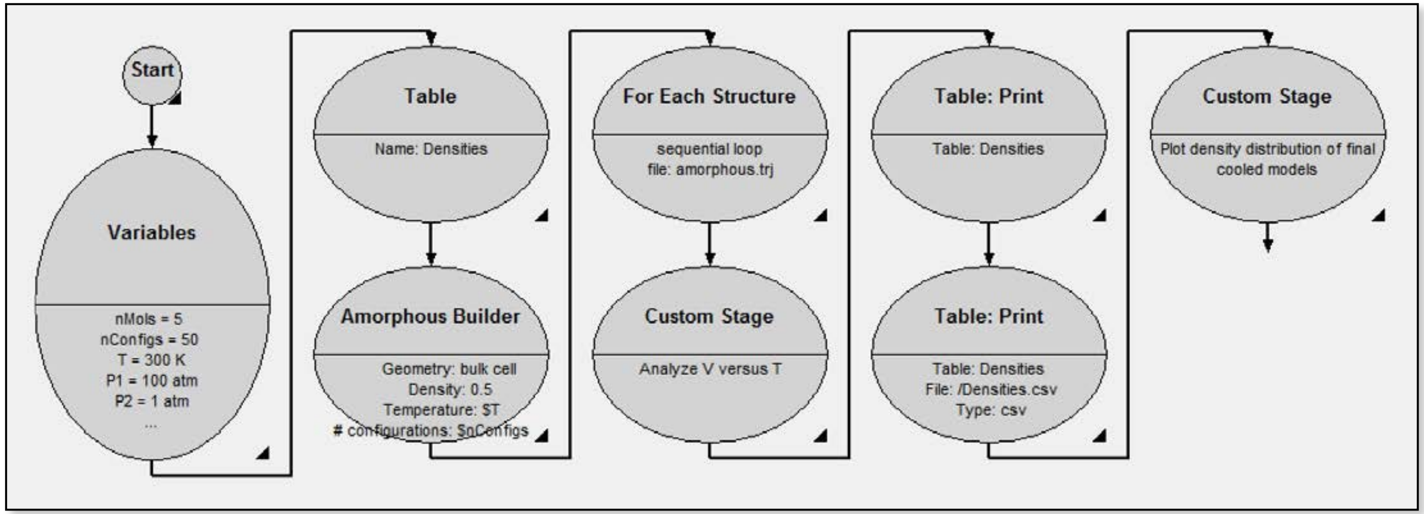
Where is the transition?

Température de Transition Vitreuse (T_g) d'un Polymère



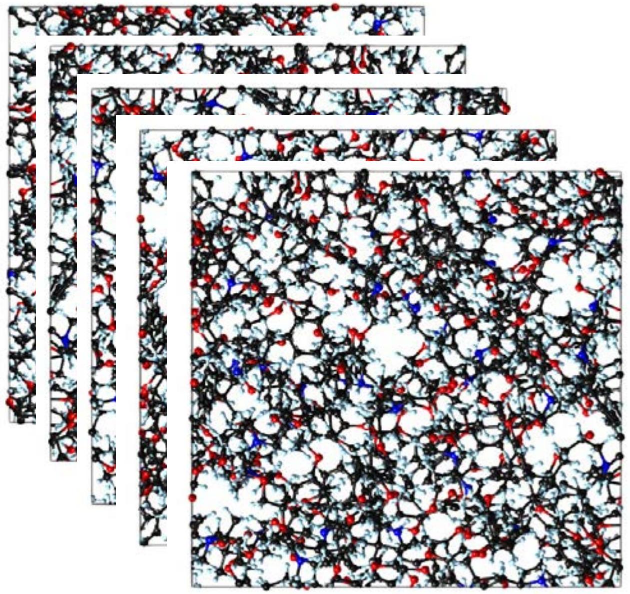
Value of high throughput calculations:

- 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



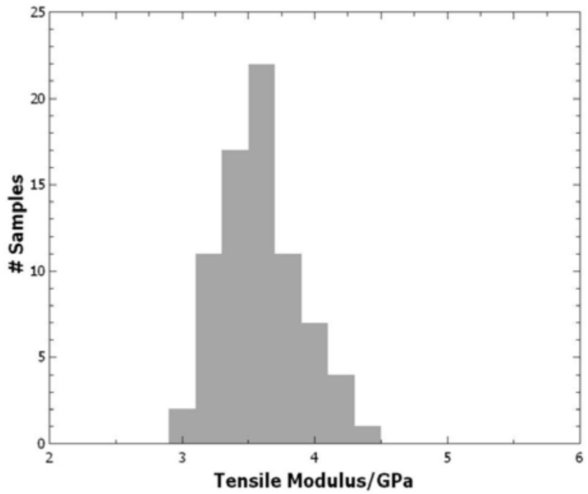


Figure 12. Distibution of tensile moduli of a batch of crosslinked DGEBA-DDS thermoset models.

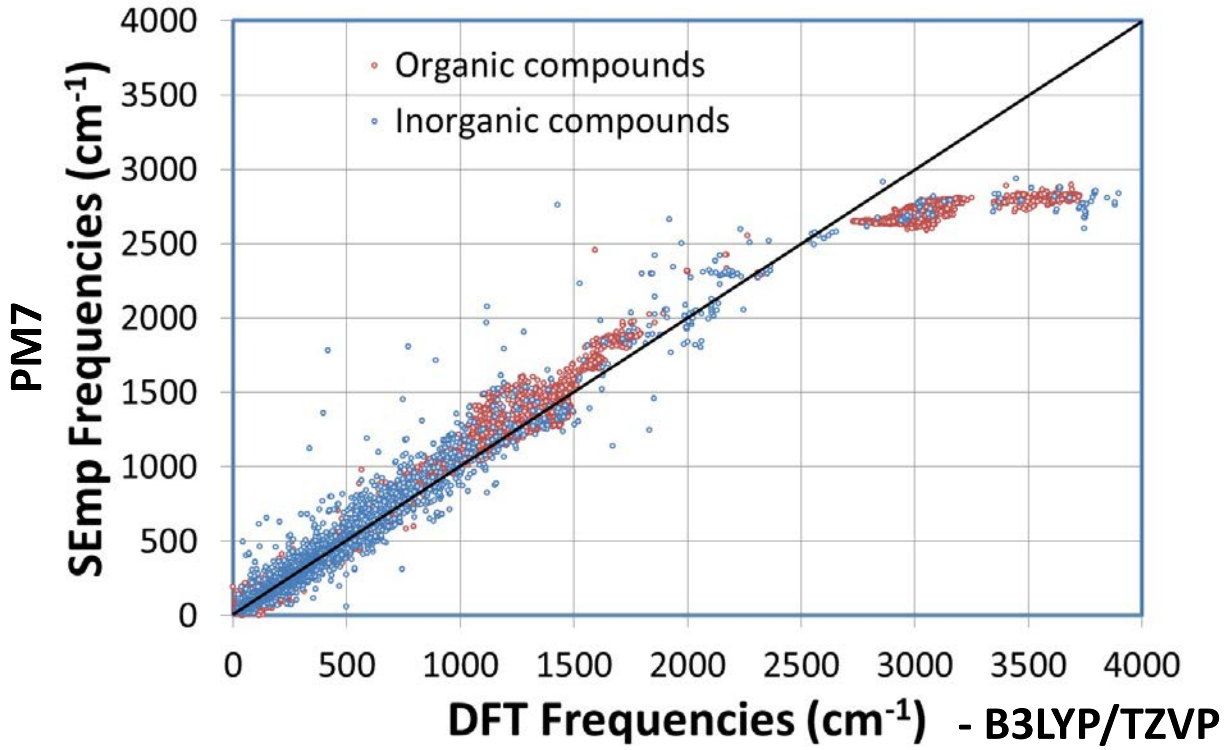
Resin	Calculated (GPa)	Experiment (GPa)	Ref.
DGEBA	3.49-3.53	2.4±.15-3.2±.15	17
TGAP	4.42-4.45	4.396±.027	18
TGDDM	5.18-5.19	5.103±.033	18

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

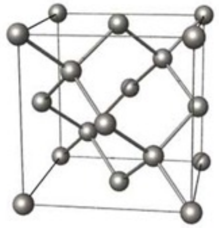


Rozanska *et al.* *J. Chem. Eng. Data* **2014**, *59*, 3136-3143 & *Oil Gas Sci. Tech*. **2015**, 70, 405-417

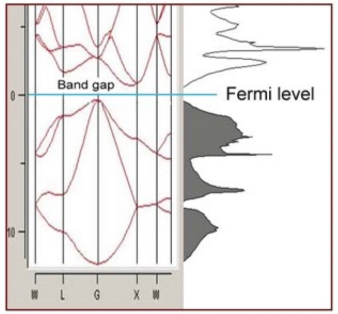
Calculs à Haut Débit

Calculs à Haut Débit

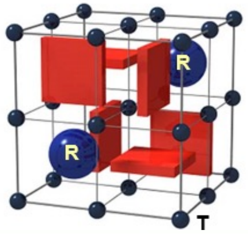
Serial

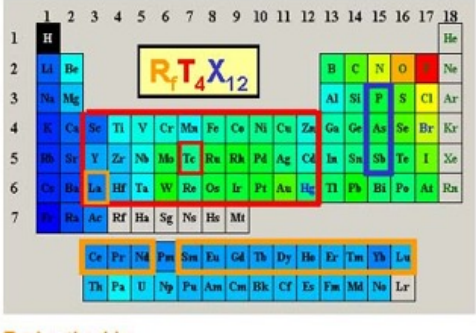


Computation

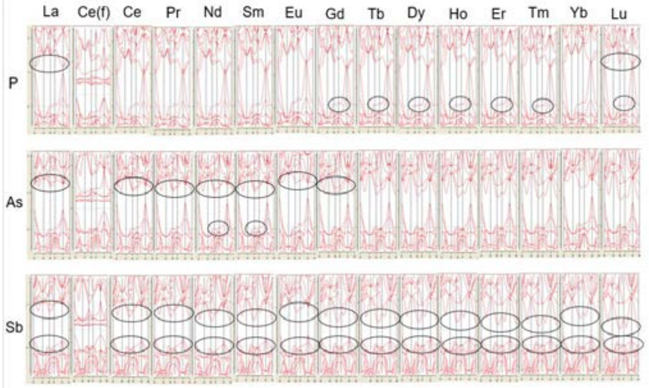


High Throughput

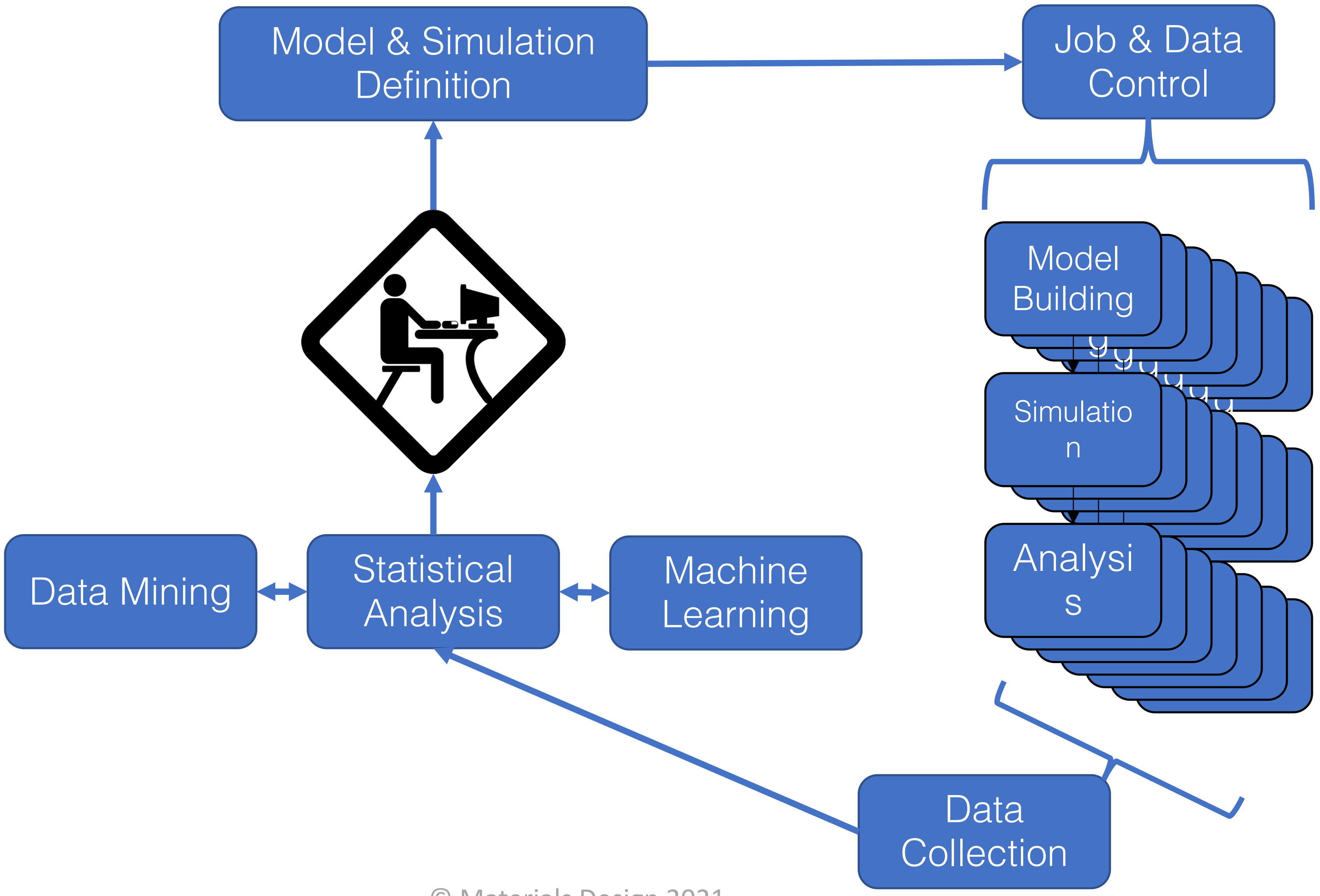




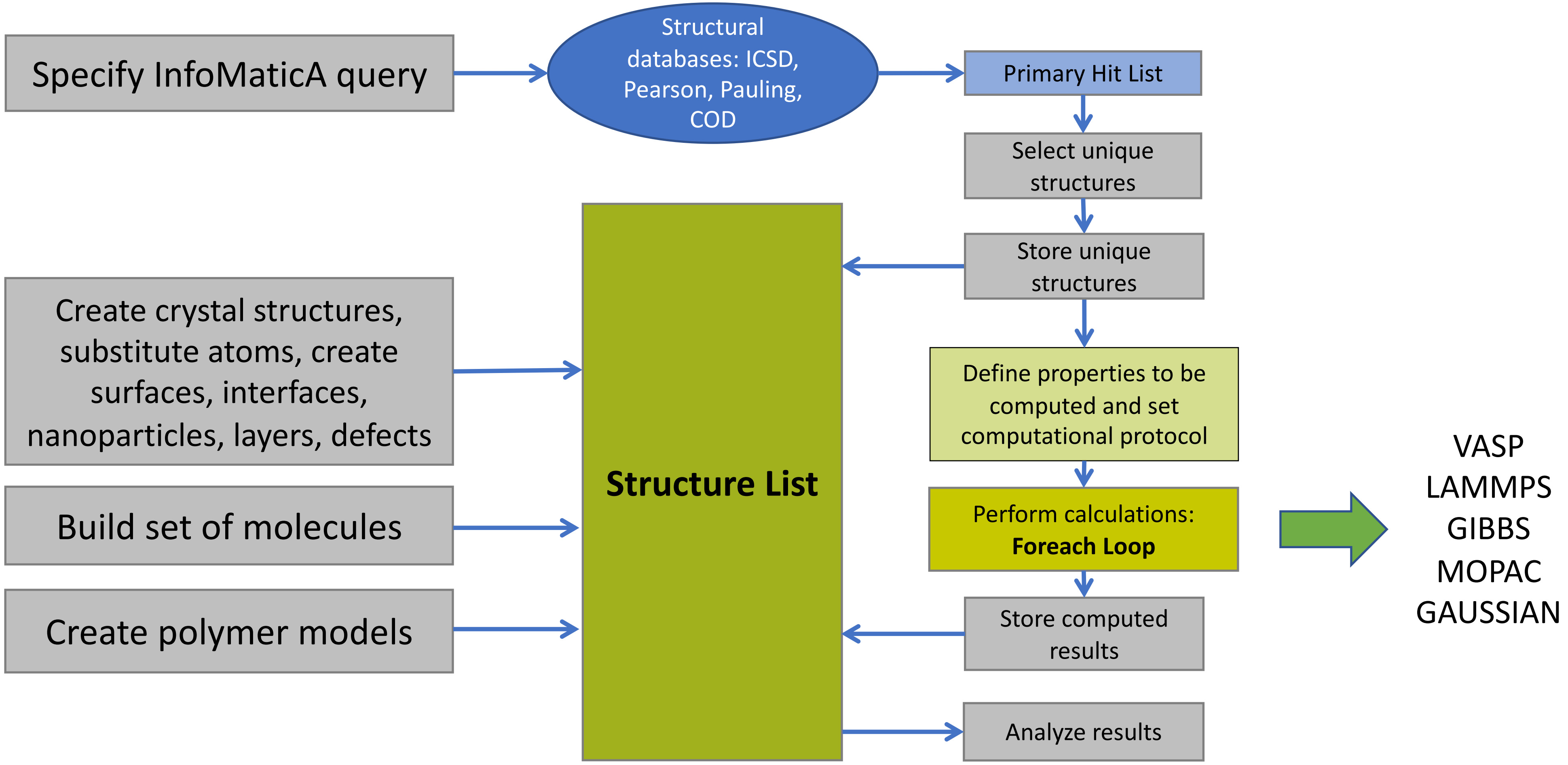
Computation



Flux des Tâches



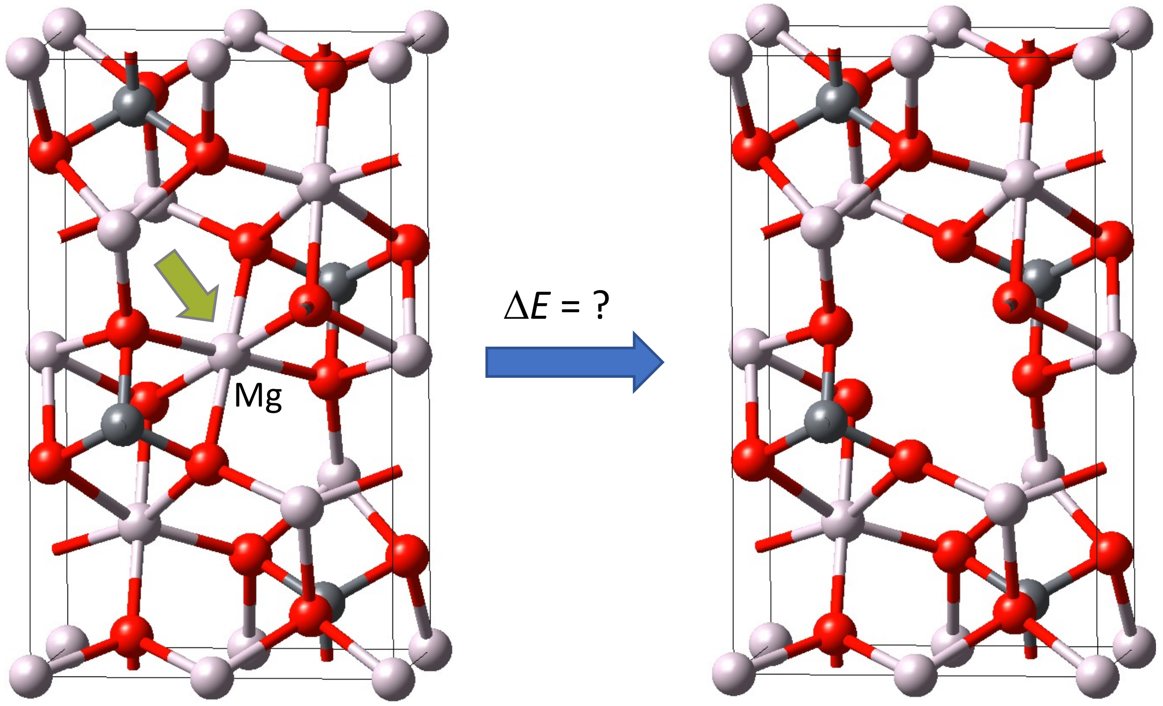
Mise en Œuvre du Calcul Haut Débit dans *MedeA*



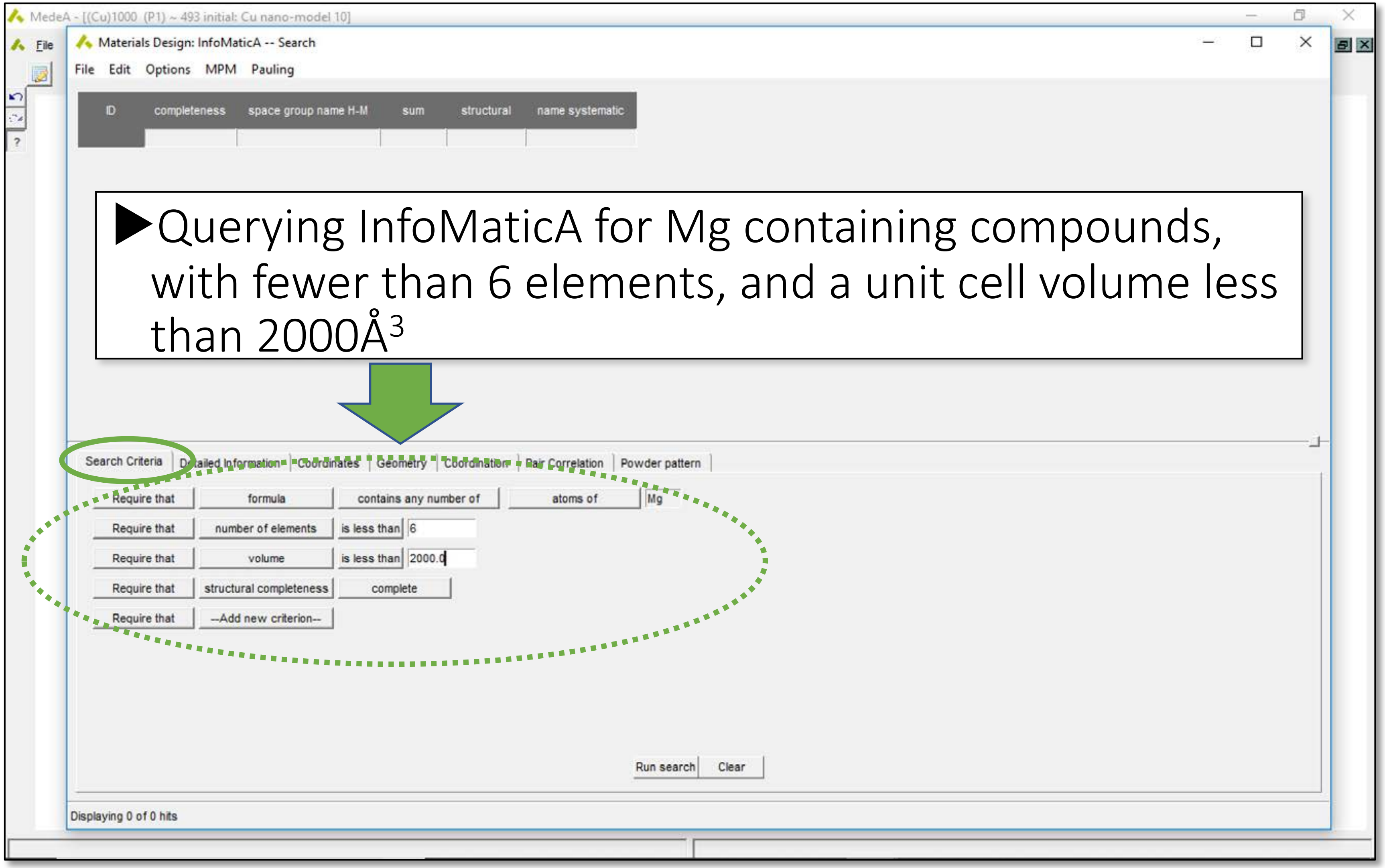
Un Calcul à Haut Débit en Pratique

Énergies de Liaison d’Atome de Magnésium

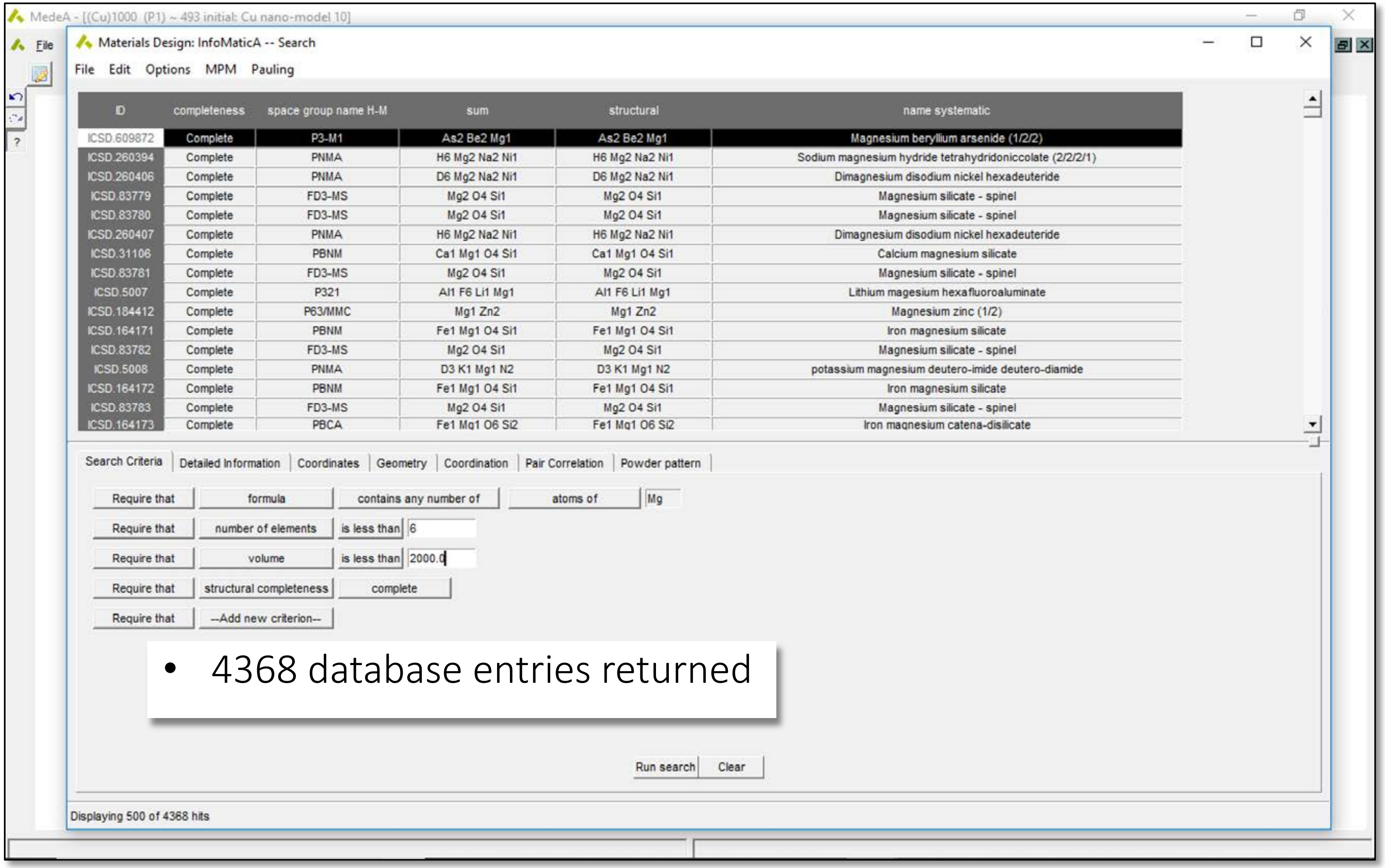
- How strongly is Mg bonded in known Mg-containing compounds?



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



Résultats de la Recherche

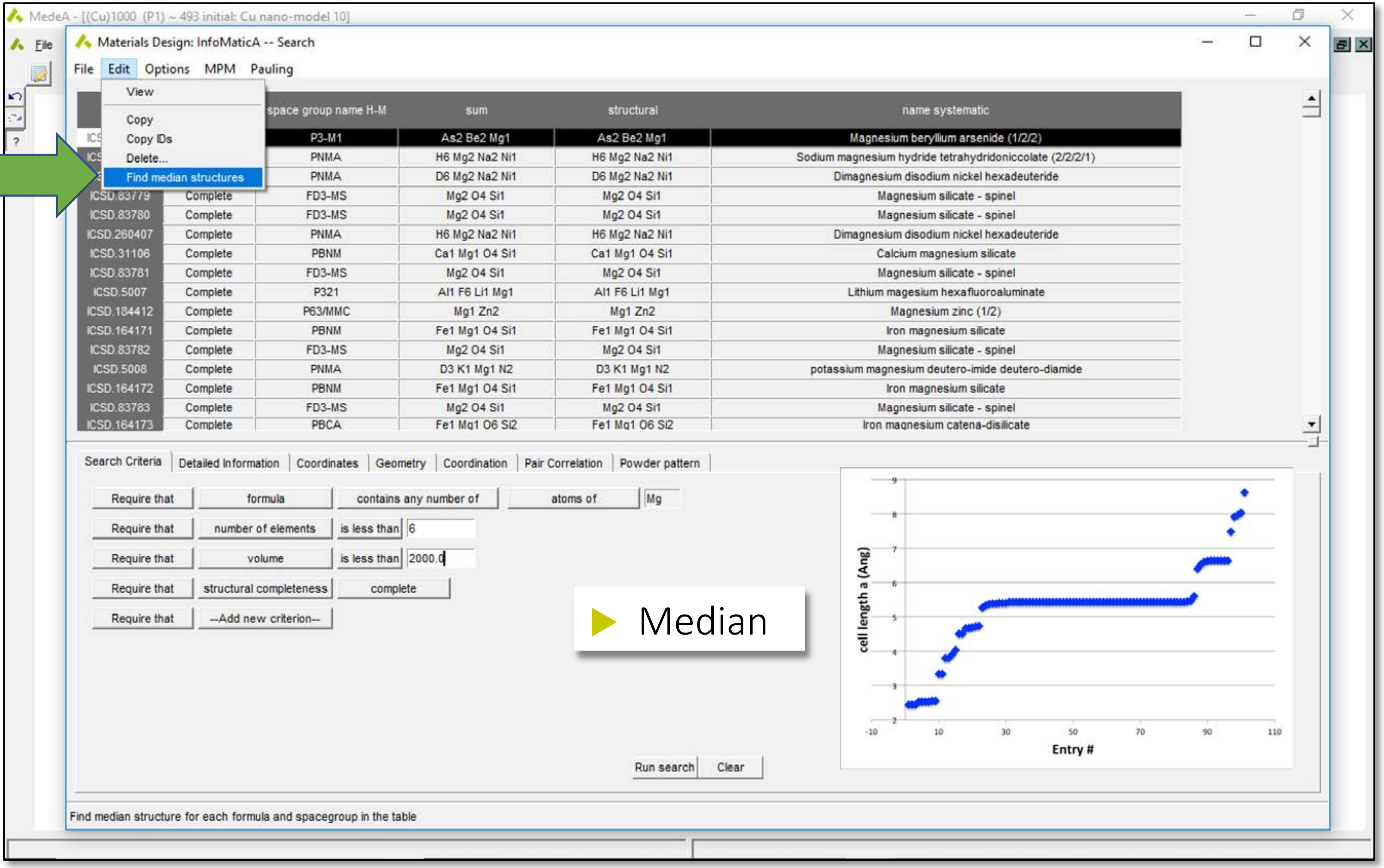


ID	completeness	space group name H-M	sum	structural	name systematic
ICSD.609872	Complete	P3-M1	As2 Be2 Mg1	As2 Be2 Mg1	Magnesium beryllium arsenide (1/2/2)
ICSD.260394	Complete	PNMA	H6 Mg2 Na2 Ni1	H6 Mg2 Na2 Ni1	Sodium magnesium hydride tetrahydridoniccolate (2/2/2/1)
ICSD.260406	Complete	PNMA	D6 Mg2 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 magesium 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 deutero-imide deutero-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 Mg1 O6 Si2	Fe1 Mg1 O6 Si2	Iron magnesium catena-disilicate

- 4368 database entries returned

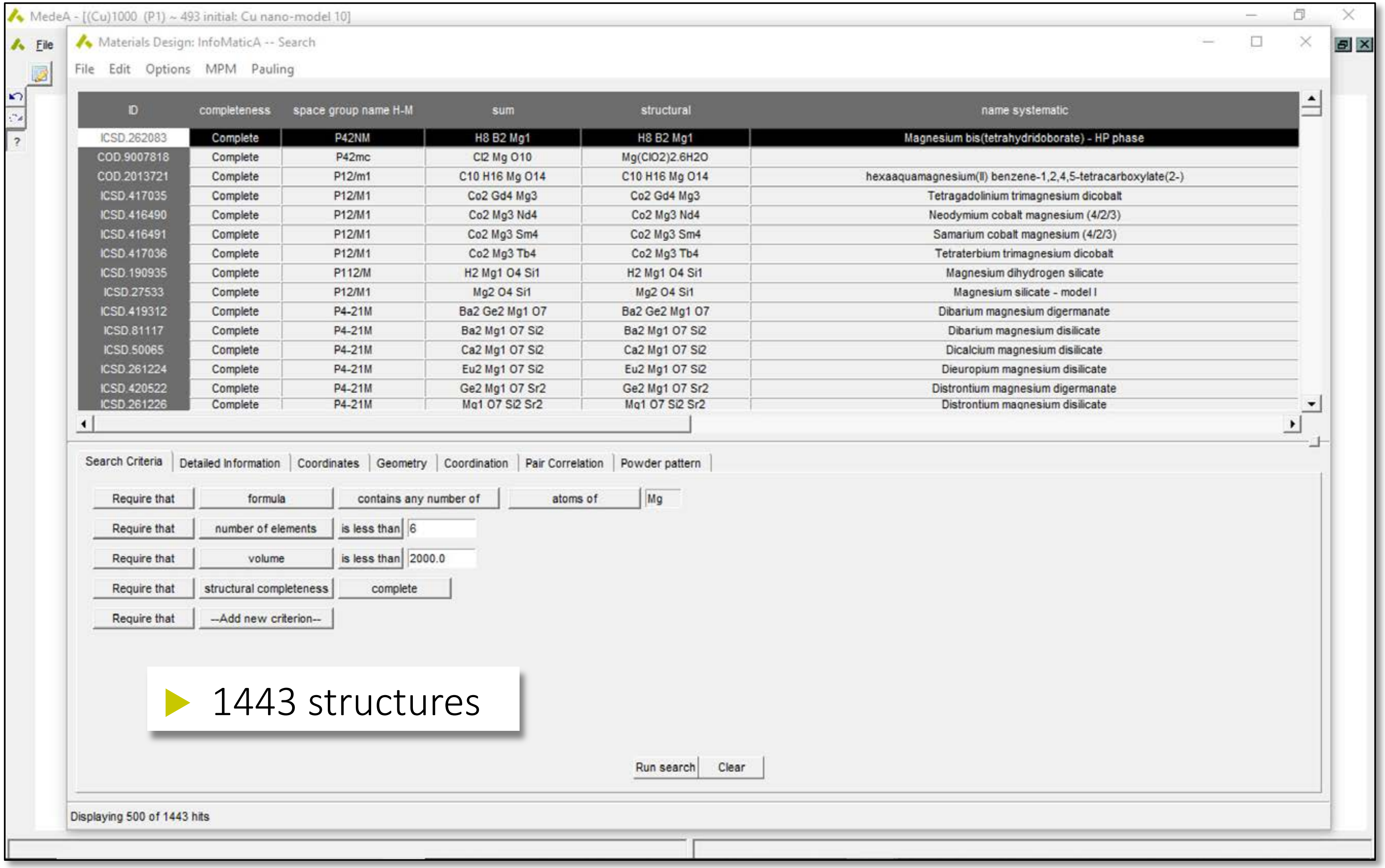
Élimination des Structures Redondantes

‘Find median structures’ command retains representative structures…



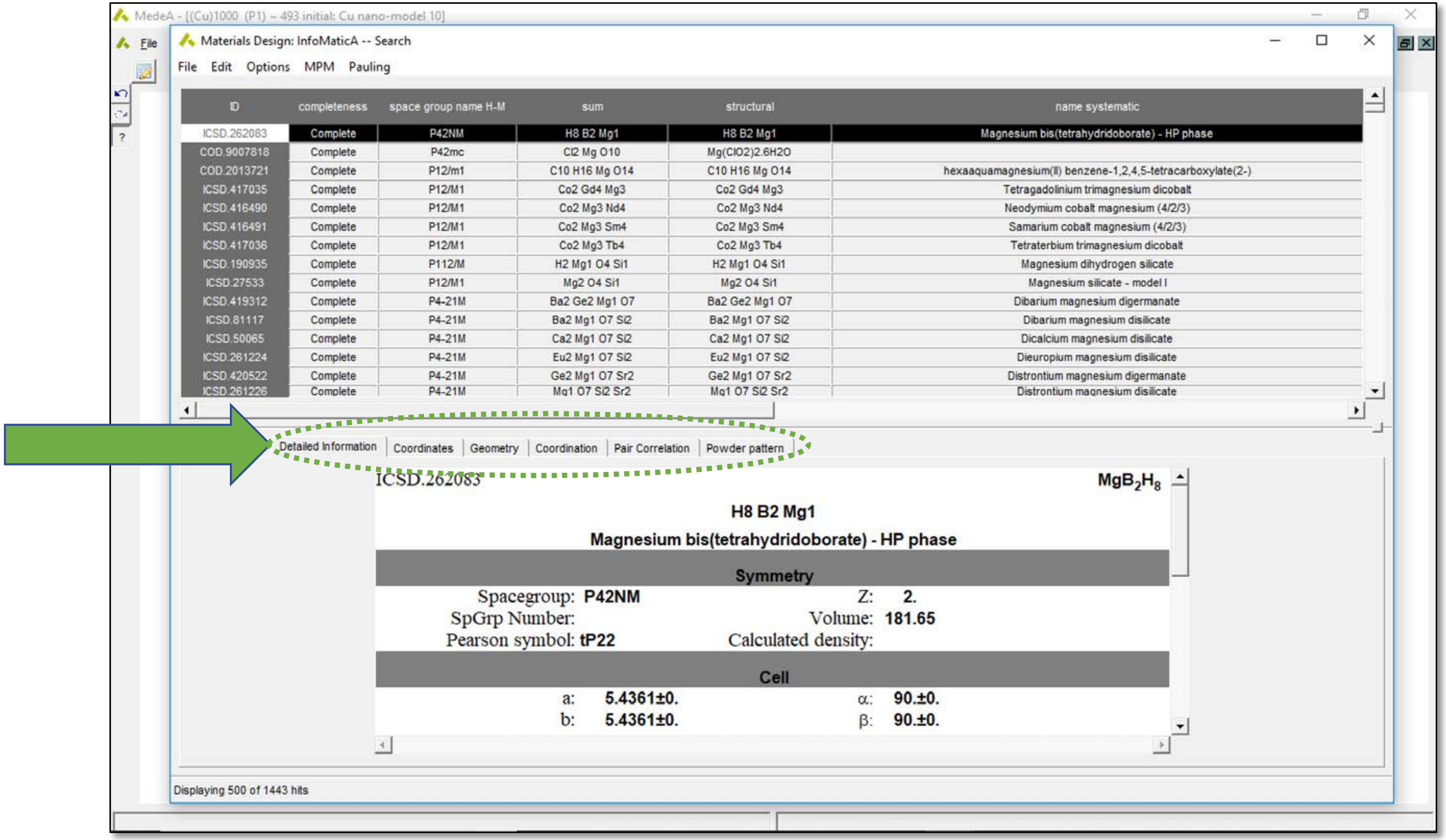
Liste de Structures Réduite

This yields 1443 structures for further analysis and computation



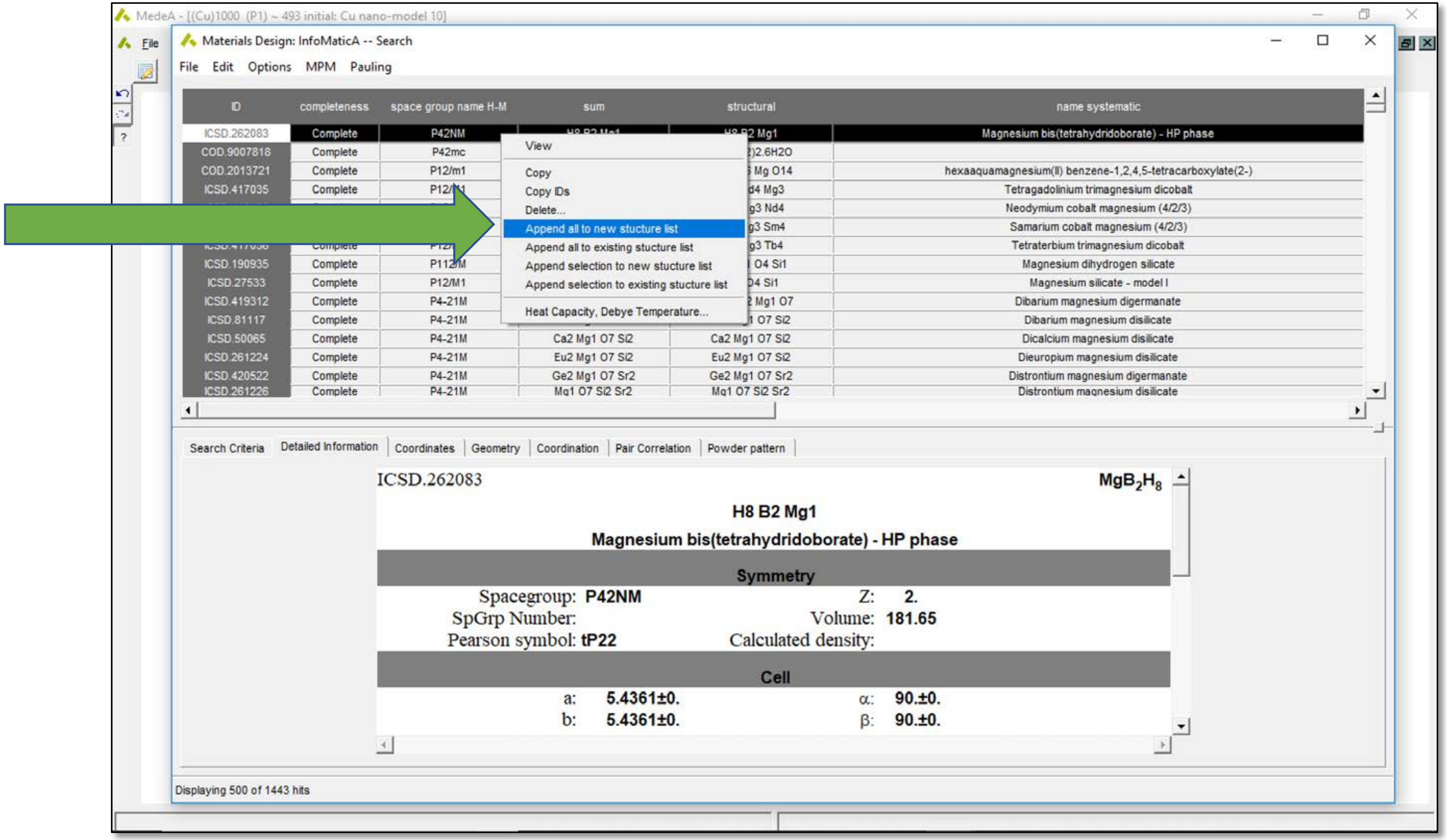
Revue des Données de la Liste de Structures

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

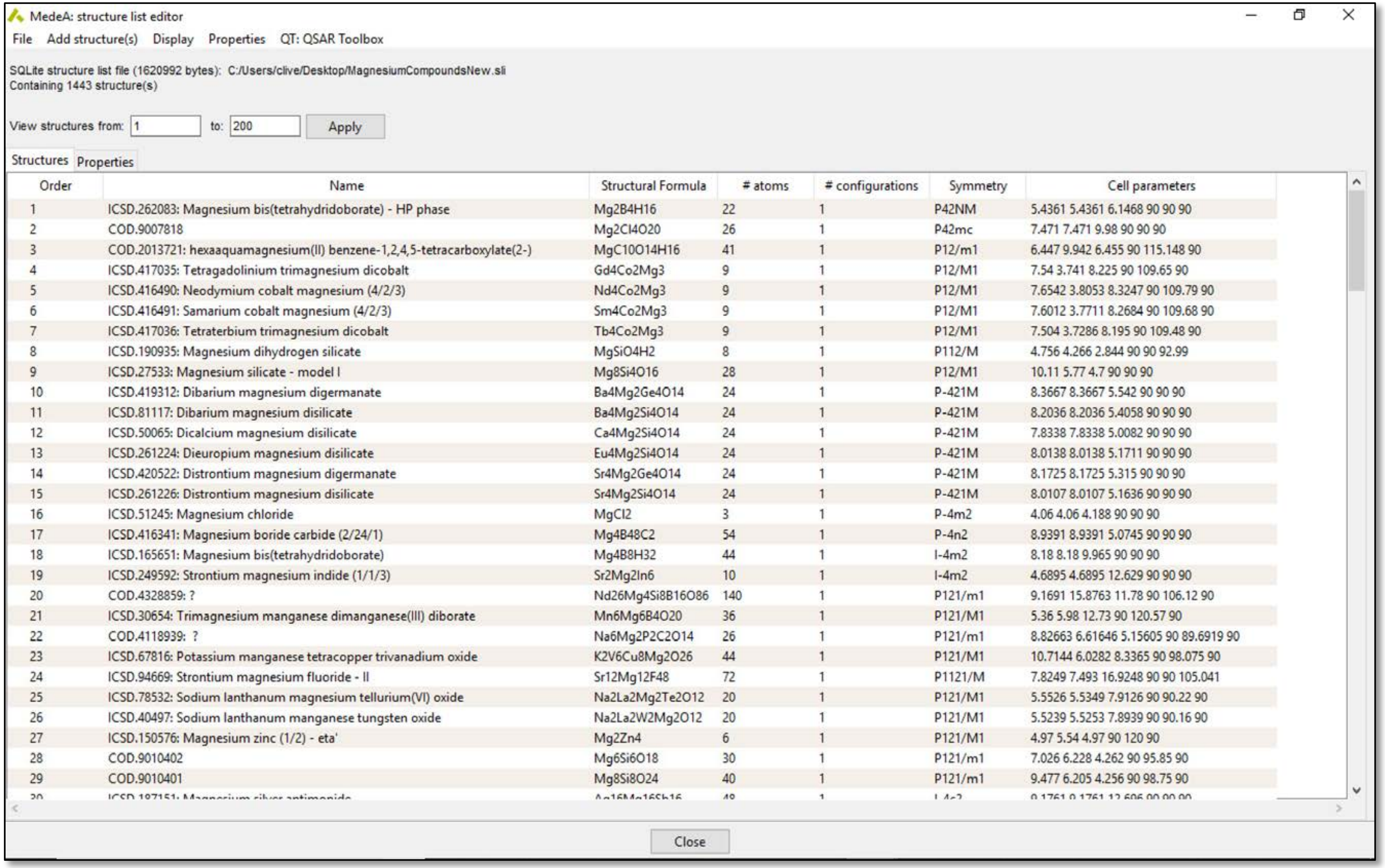


Sauvegarde de la Liste de Structures

The refined list is saved directly as a structure list



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: 1 to: 200 Apply

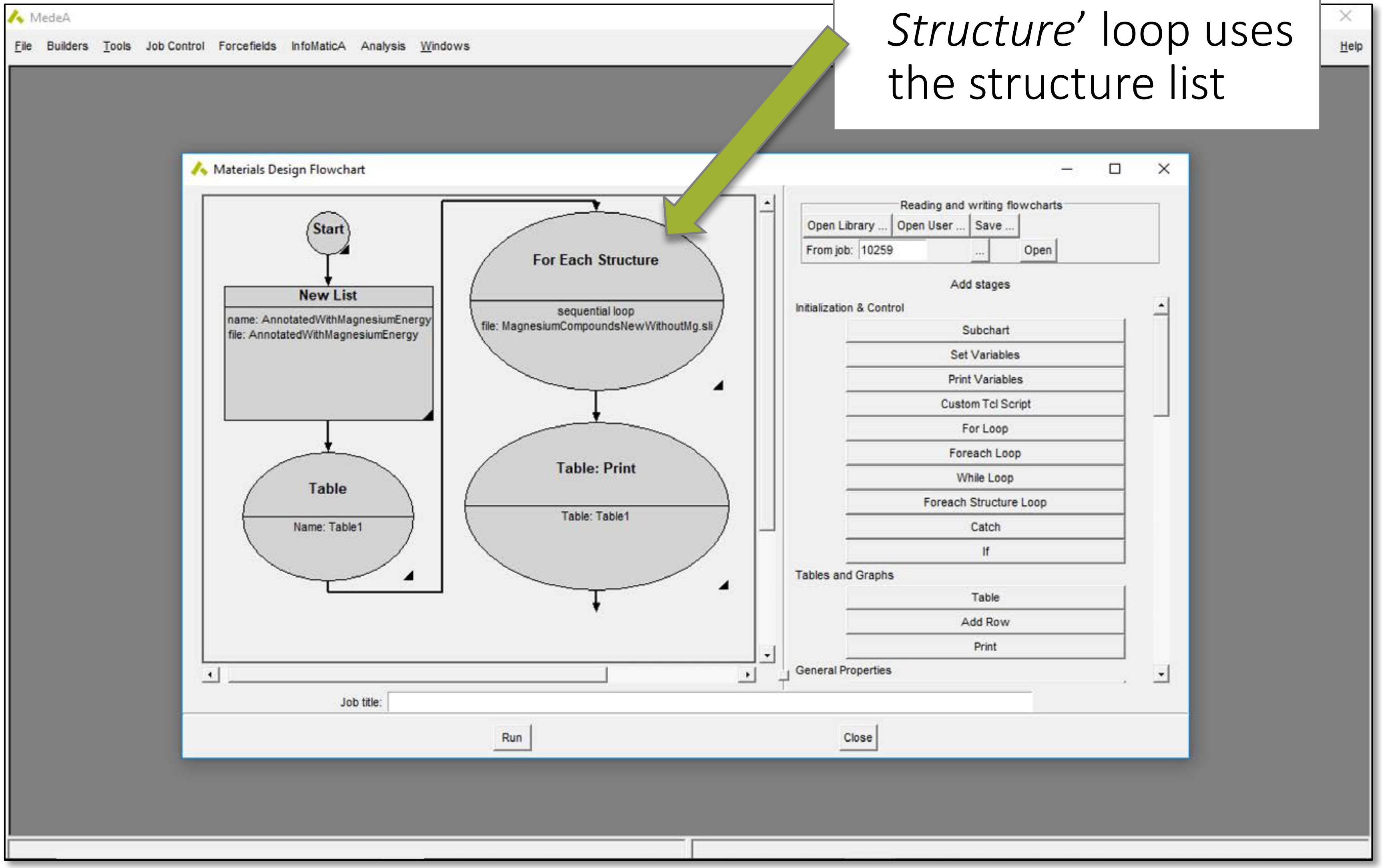
Structures | Properties

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.187151: Magnesium silver antimonide	Ag16Mg16Sb16	48	1	I-4c2	9.1761 9.1761 12.696 90 90 90

Close

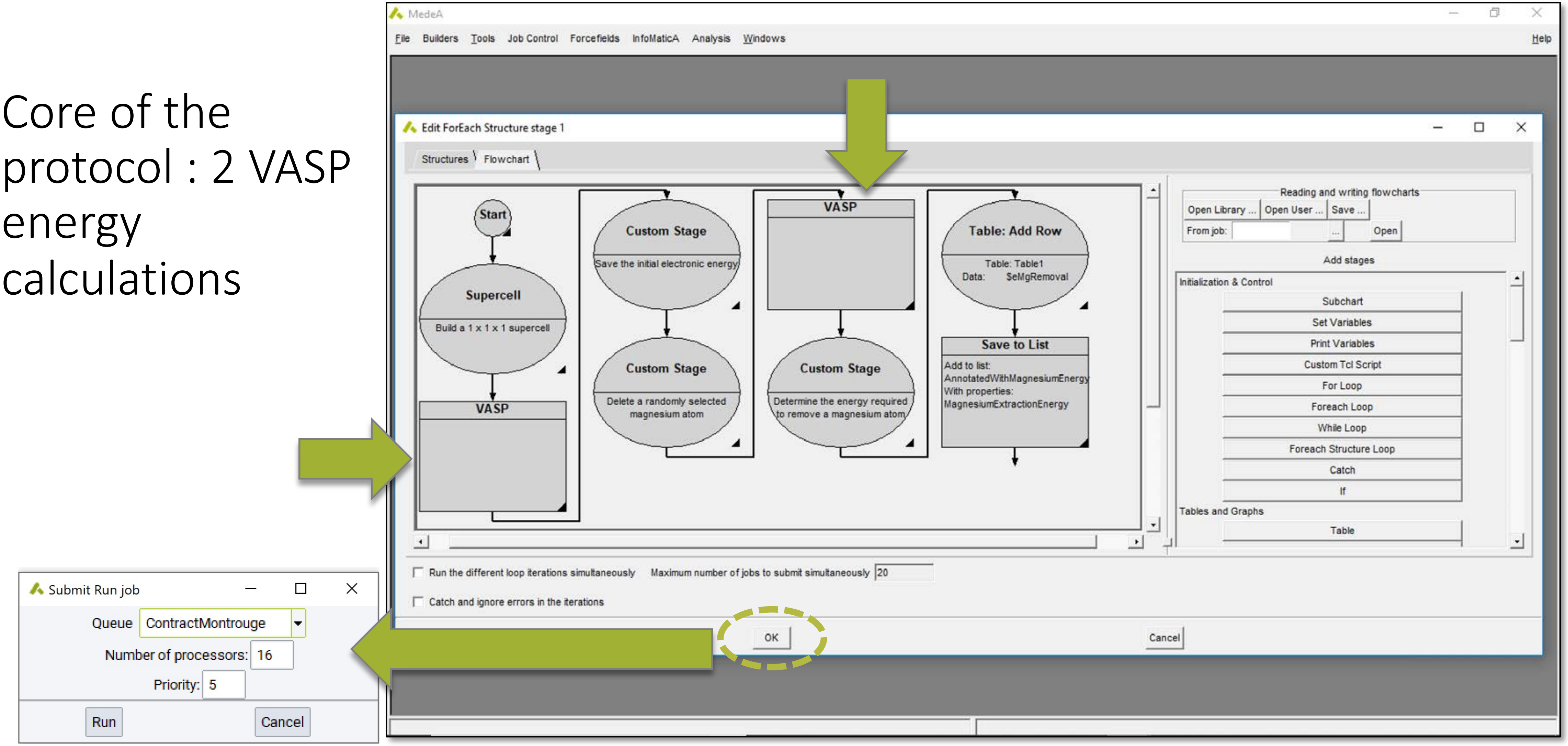
Organigramme des Tâches du Calcul du Potentiel Chimique du Magnésium

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



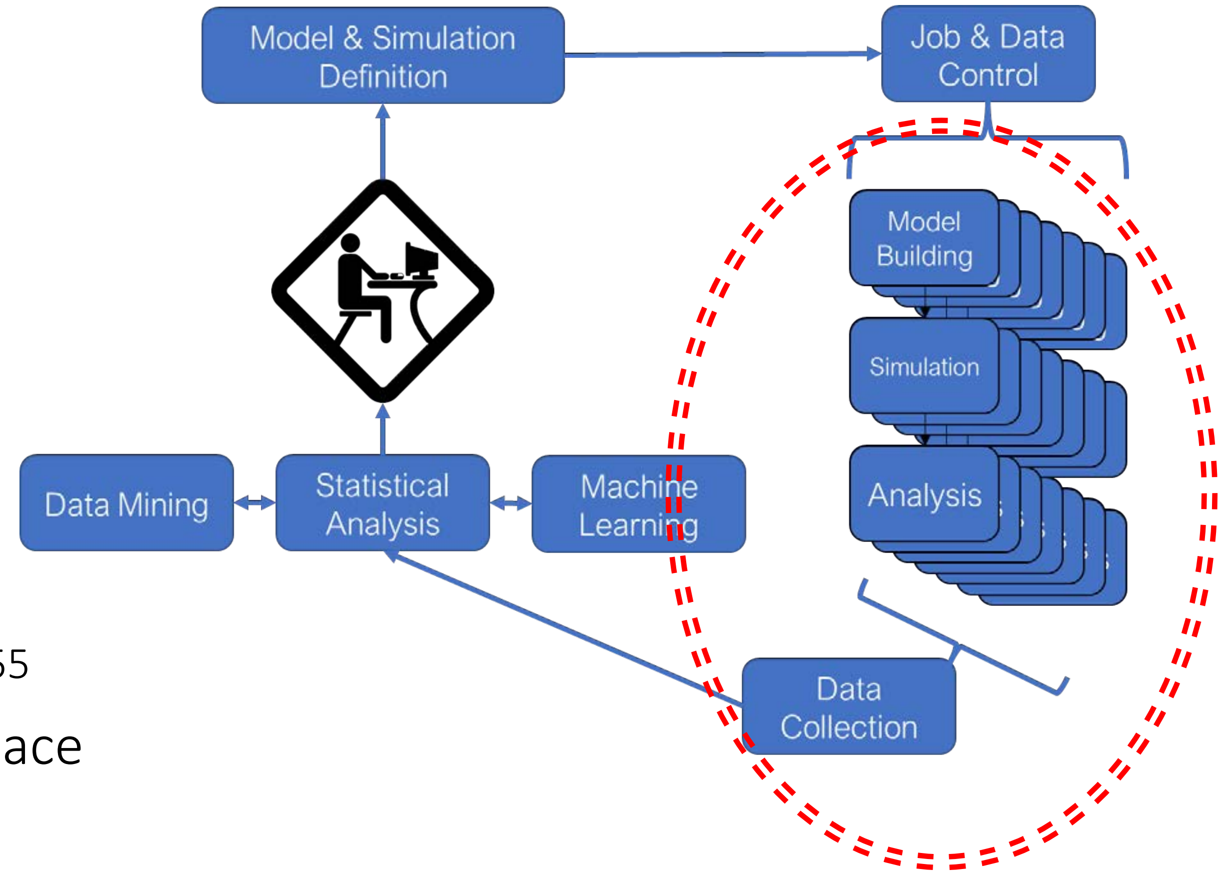
Détails du Protocol du Calcul pour le Magnésium

- Core of the protocol : 2 VASP energy calculations



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

MedeA: structure list editor

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

SQLite structure list file (8258560 bytes): C:/Users/clive/Desktop/AnnotatedWithMagnesiumEnergy1.sli
Containing 1442 structure(s)

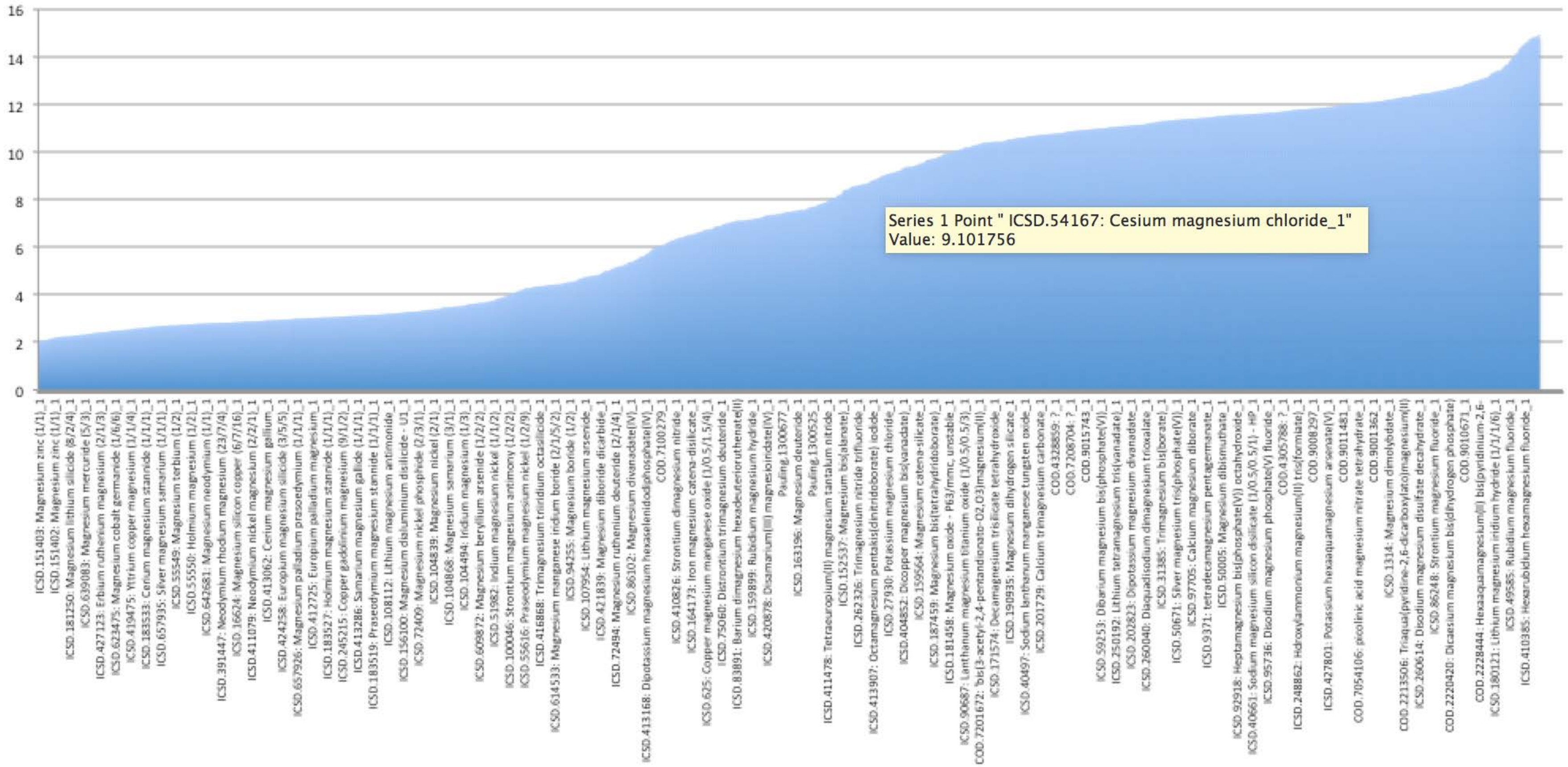
View structures from: 1 to: 1442 Apply

Structures | Properties

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	9.0767079999999964
2	COD.9007818_1	Mg2Cl4O20	26	1	P1	7.471 7.471 9.98 90 90 90	11.678332999999995
3	COD.2013721: hexaaquamagnesium(II) benzene-1,2,4,5-tetracarbc	MgC10O14H16	41	1	P1	6.447 9.942 6.455 90 115.148 90	13.024231999999984
4	ICSD.417035: Tetragadolinium trimagnesium dicobalt_1	Gd4Co2Mg3	9	1	P1	7.54 3.741 8.225 90 109.65 90	2.6571440000000024
5	ICSD.416490: Neodymium cobalt magnesium (4/2/3)_1	Nd4Co2Mg3	9	1	P1	7.6542 3.8053 8.3247 90 109.79 90	2.6206330000000051
6	ICSD.416491: Samarium cobalt magnesium (4/2/3)_1	Sm4Co2Mg3	9	1	P1	7.6012 3.7711 8.2684 90 109.68 90	2.6354080000000053
7	ICSD.417036: Tetraterbium trimagnesium dicobalt_1	Tb4Co2Mg3	9	1	P1	7.504 3.7286 8.195 90 109.48 90	2.6607569999999967
8	ICSD.190935: Magnesium dihydrogen silicate_1	MgSiO4H2	8	1	P1	4.756 4.266 2.844 90 90 92.99	10.541487000000004
9	ICSD.27533: Magnesium silicate - model I_1	Mg8Si4O16	28	1	P1	10.11 5.77 4.7 90 90 90	10.080409000000003
10	ICSD.419312: Dibarium magnesium digermanate_1	Ba4Mg2Ge4O14	24	1	P1	8.3667 8.3667 5.542 90 90 90	11.347779999999972
11	ICSD.81117: Dibarium magnesium disilicate_1	Ba4Mg2Si4O14	24	1	P1	8.2036 8.2036 5.4058 90 90 90	11.337536999999998
12	ICSD.50065: Dicalcium magnesium disilicate_1	Ca4Mg2Si4O14	24	1	P1	7.8338 7.8338 5.0082 90 90 90	11.511885000000007
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	11.391487999999981
15	ICSD.261226: Distrontium magnesium disilicate_1	Sr4Mg2Si4O14	24	1	P1	8.0107 8.0107 5.1636 90 90 90	11.467181000000011
16	ICSD.51245: Magnesium chloride_1	MgCl2	3	1	P1	4.06 4.06 4.188 90 90 90	8.6441009999999991
17	ICSD.416341: Magnesium boride carbide (2/24/1)_1	Mg4B48C2	54	1	P1	8.9391 8.9391 5.0745 90 90 90	4.5614679999999908
18	ICSD.165651: Magnesium bis(tetrahydridoborate)_1	Mg4B8H32	44	1	P1	8.18 8.18 9.965 90 90 90	10.287706000000014
19	ICSD.249592: Strontium magnesium indide (1/1/3)_1	Sr2Mg2In6	10	1	P1	4.6895 4.6895 12.629 90 90 90	2.587607000000002
20	COD.4328859: ?_1	Nd26Mg4Si8B16O86	140	1	P1	9.1691 15.8763 11.78 90 106.12 90	10.780890999999883
21	ICSD.30654: Trimagnesium manganese dimanganese(III) diborate	Mn6Mg6B4O20	36	1	P1	5.36 5.98 12.73 90 120.57 90	6.7704059999999799
22	COD.4118939: ?_1	Na6Mg2P2C2O14	26	1	P1	8.82663 6.61646 5.15605 90 89.6919 90	10.475797999999998
23	ICSD.67816: Potassium manganese tetracopper trivanadium oxide	K2V6Cu8Mg2O26	44	1	P1	10.7144 6.0282 8.3365 90 98.075 90	9.4981760000000008
24	ICSD.94669: Strontium magnesium fluoride - II_1	Sr12Mg12F48	72	1	P1	7.8249 7.493 16.9248 90 90 105.041	14.494196999999986
25	ICSD.78532: Sodium lanthanum magnesium tellurium(VI) oxide_1	Na2La2Mg2Te2O12	20	1	P1	5.5526 5.5349 7.9126 90 90.22 90	10.437513999999993
26	ICSD.40497: Sodium lanthanum manganese tungsten oxide_1	Na2La2W2Mg2O12	20	1	P1	5.5239 5.5253 7.8939 90 90.16 90	10.615187999999989
27	ICSD.150576: Magnesium zinc (1/2) - eta'_1	Mg2Zn4	6	1	P1	4.97 5.54 4.97 90 120 90	2.6280370000000008
28	COD.9010402_1	Mg6Si6O18	30	1	P1	7.026 6.228 4.262 90 95.85 90	7.3878770000000031
29	COD.9010401_1	Mg8Si8O24	40	1	P1	9.477 6.205 4.256 90 98.75 90	7.2147510000000068

Close

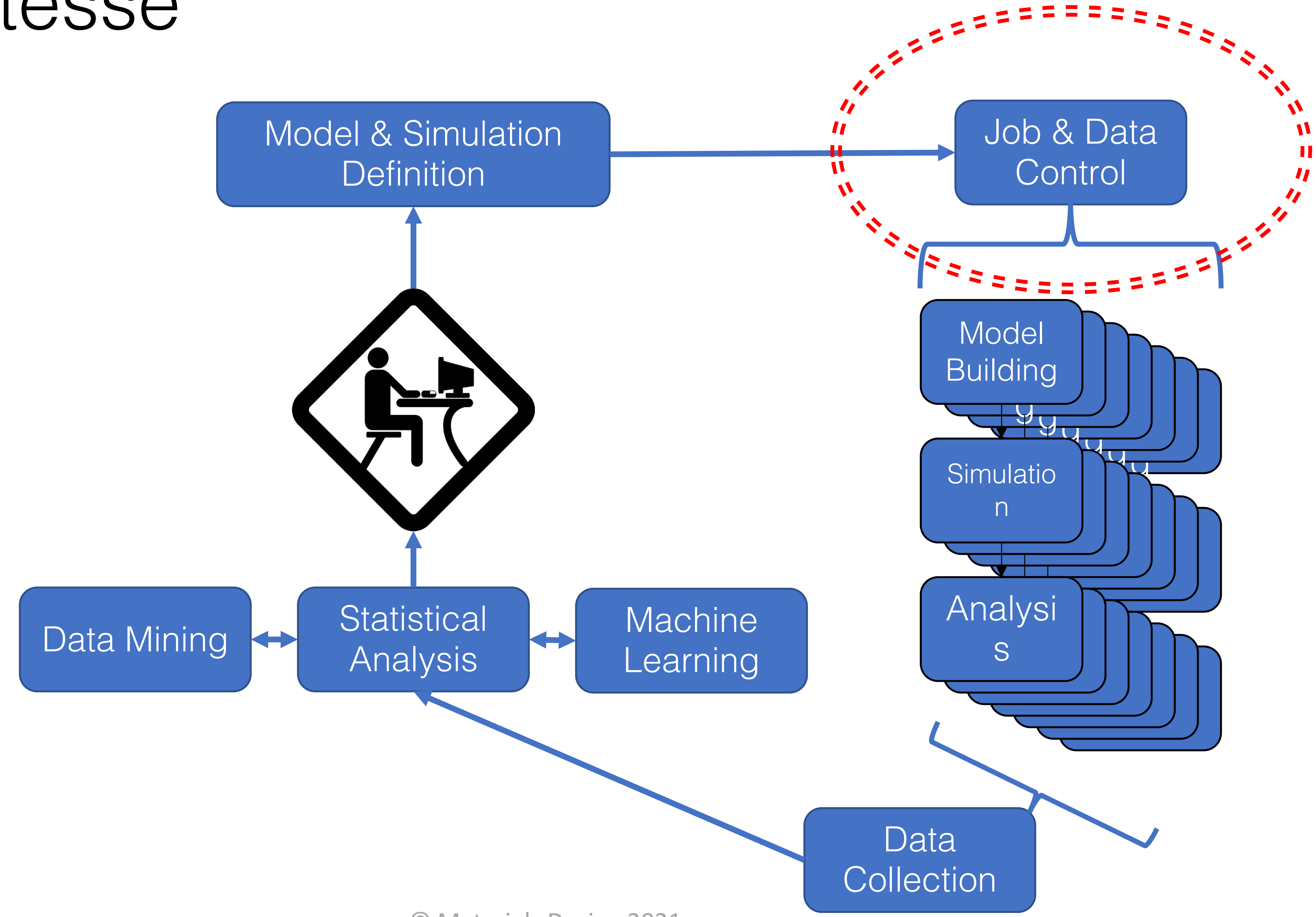
Énergies de Liaison du Magnésium



- Ranking of the magnesium removal energies

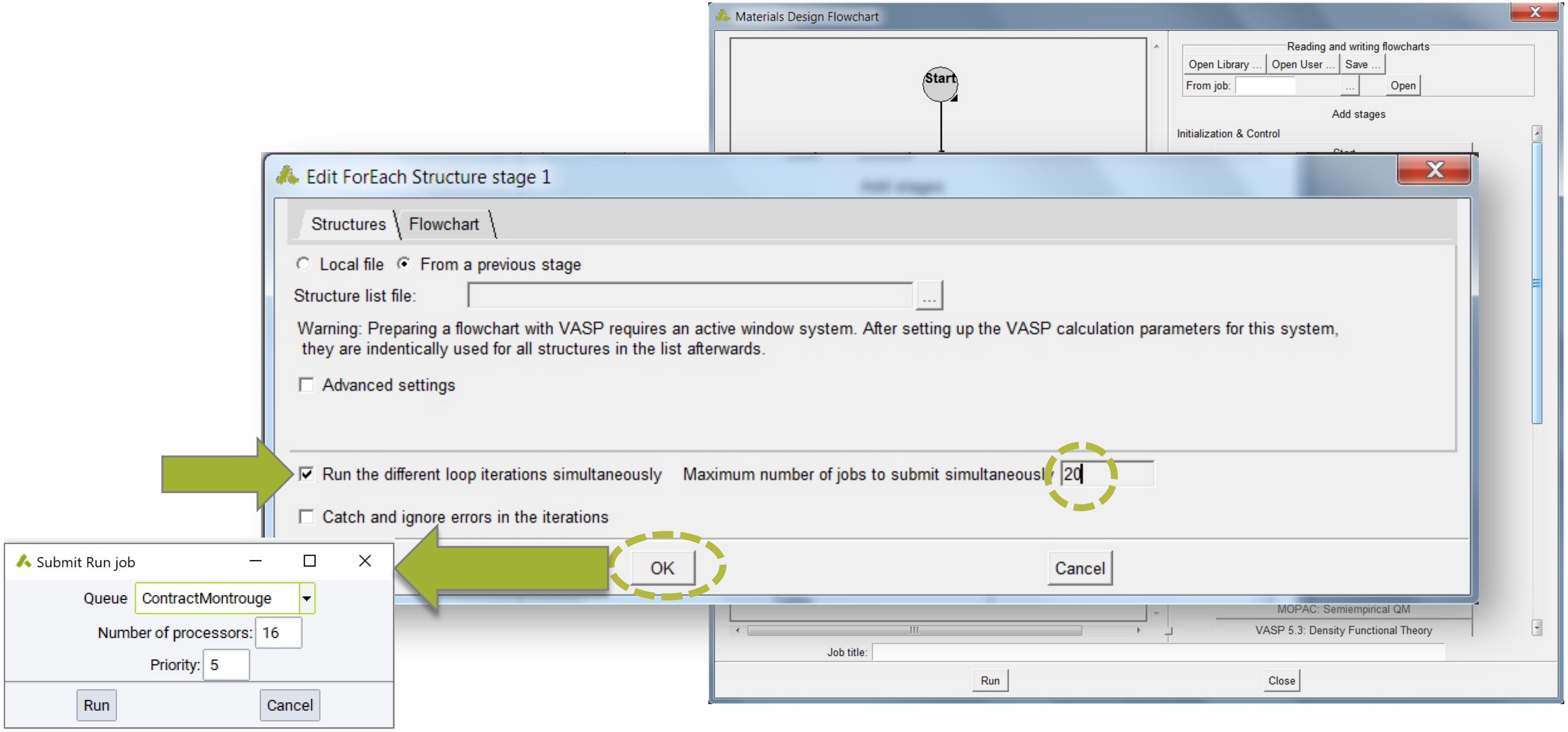
Infrastructure et Calculs Haut Débit dans *MedeA* : Atouts, Robustesse et Versatilité

Robustesse



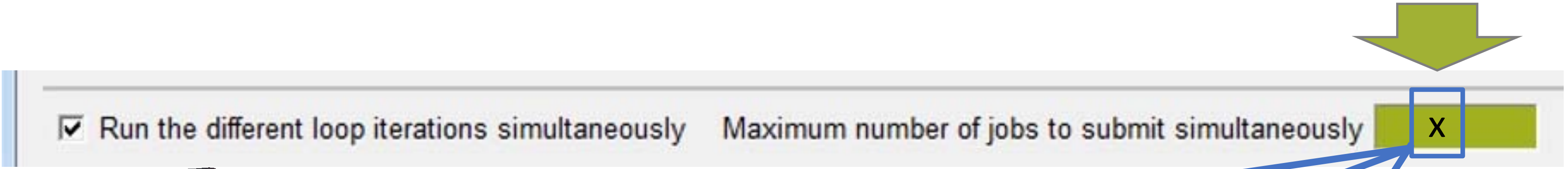
Model & Simulation Definition
Job & Data Control
Model Building
Simulatio n
Analysi s
Data Mining
Statistical Analysis
Machine Learning
Data Collection

Mise en Œuvre du Calcul Haut Débit dans *MedeA*



- Value: Highly efficient screening of large number of compounds

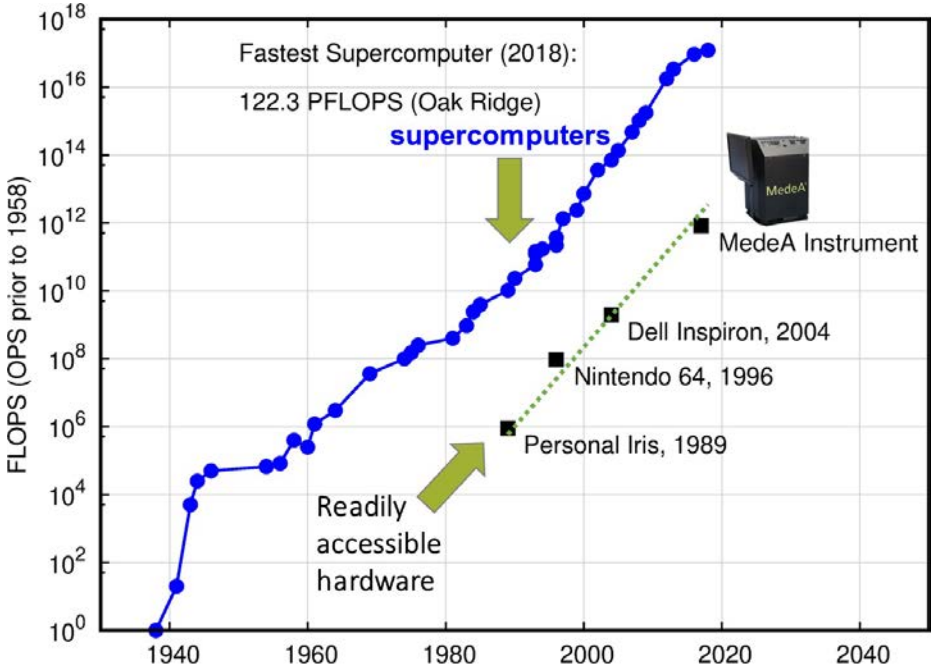
Mise en Œuvre du Calcul Haut Débit dans *MedeA*



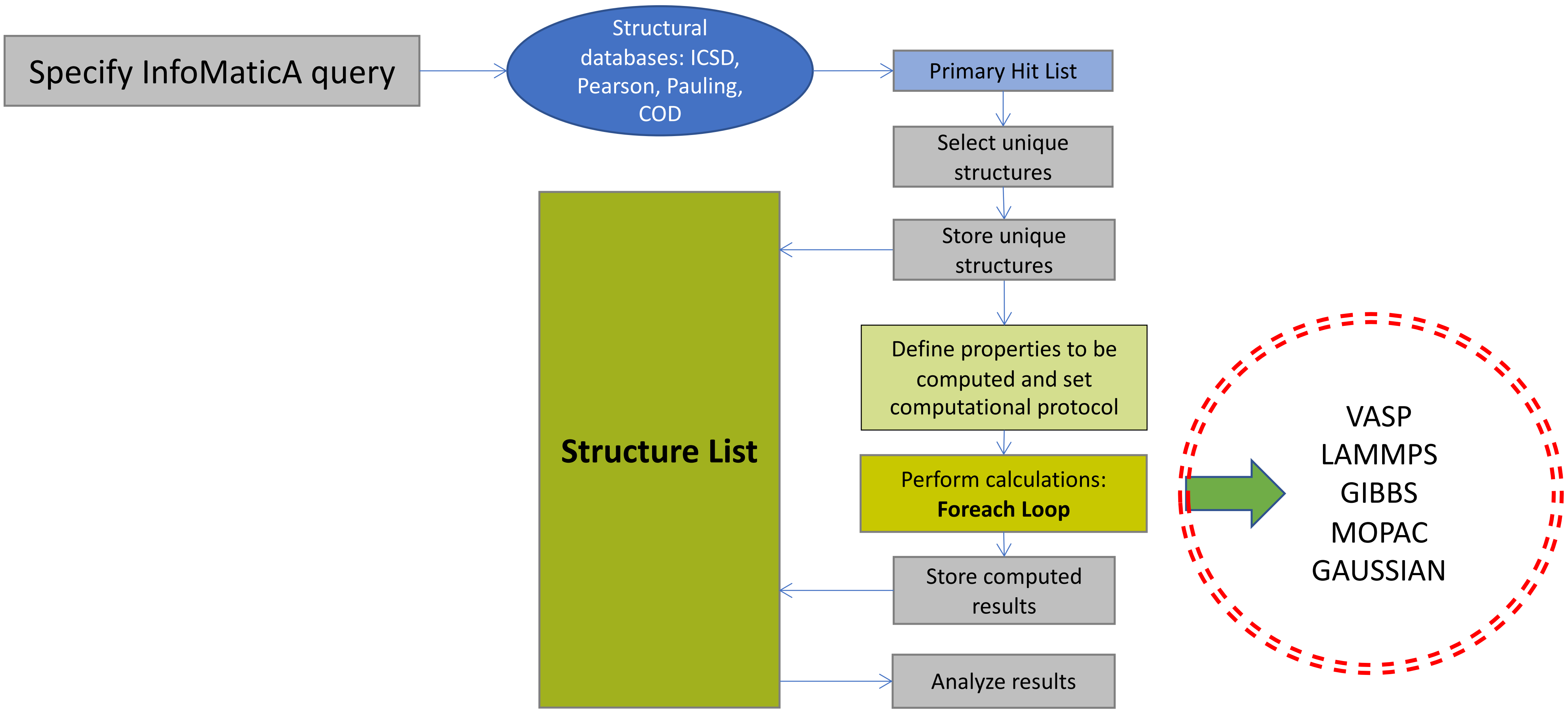
4 jobs×1 core

10 jobs×8-16 cores

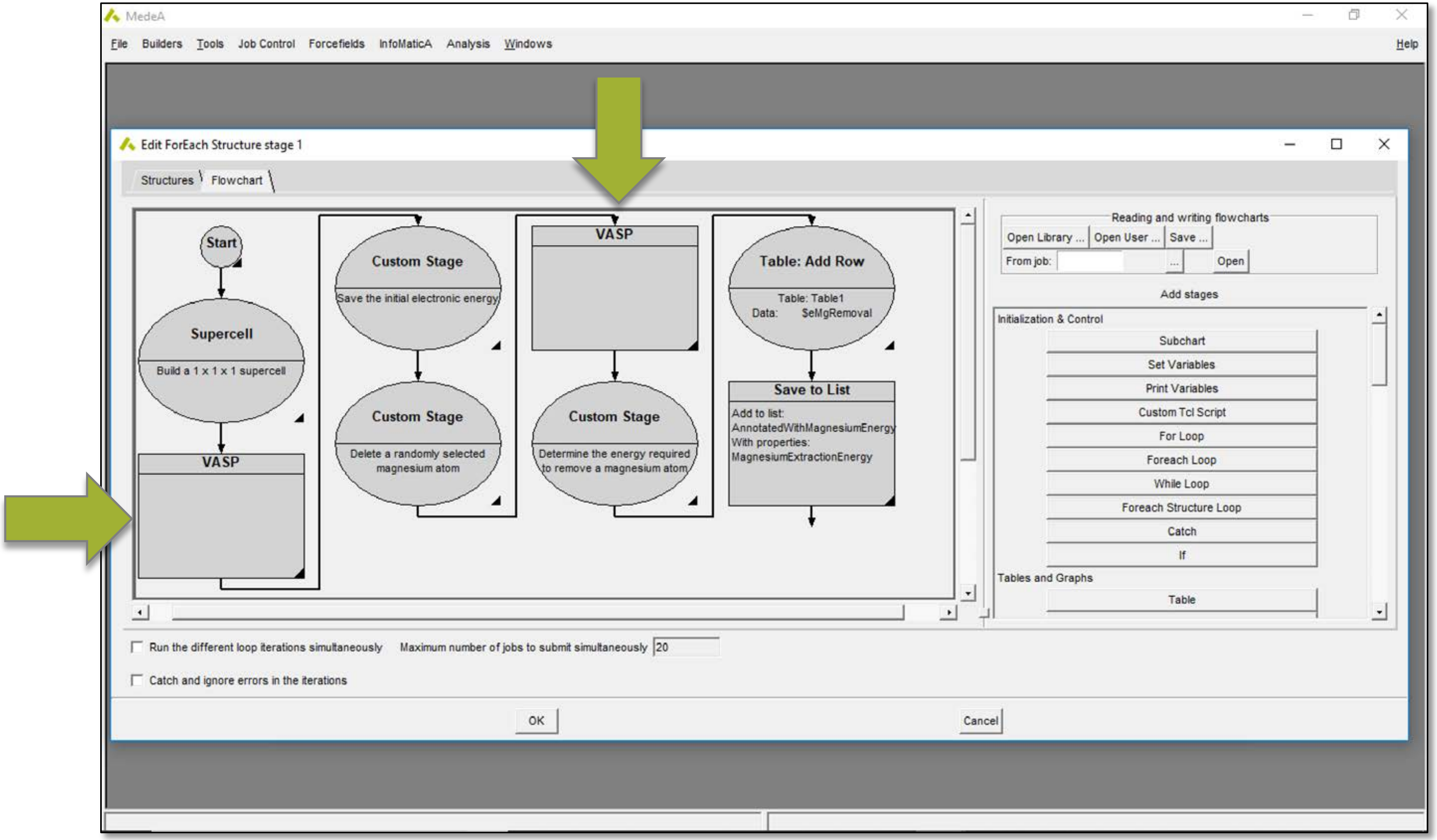
100 jobs×32 cores



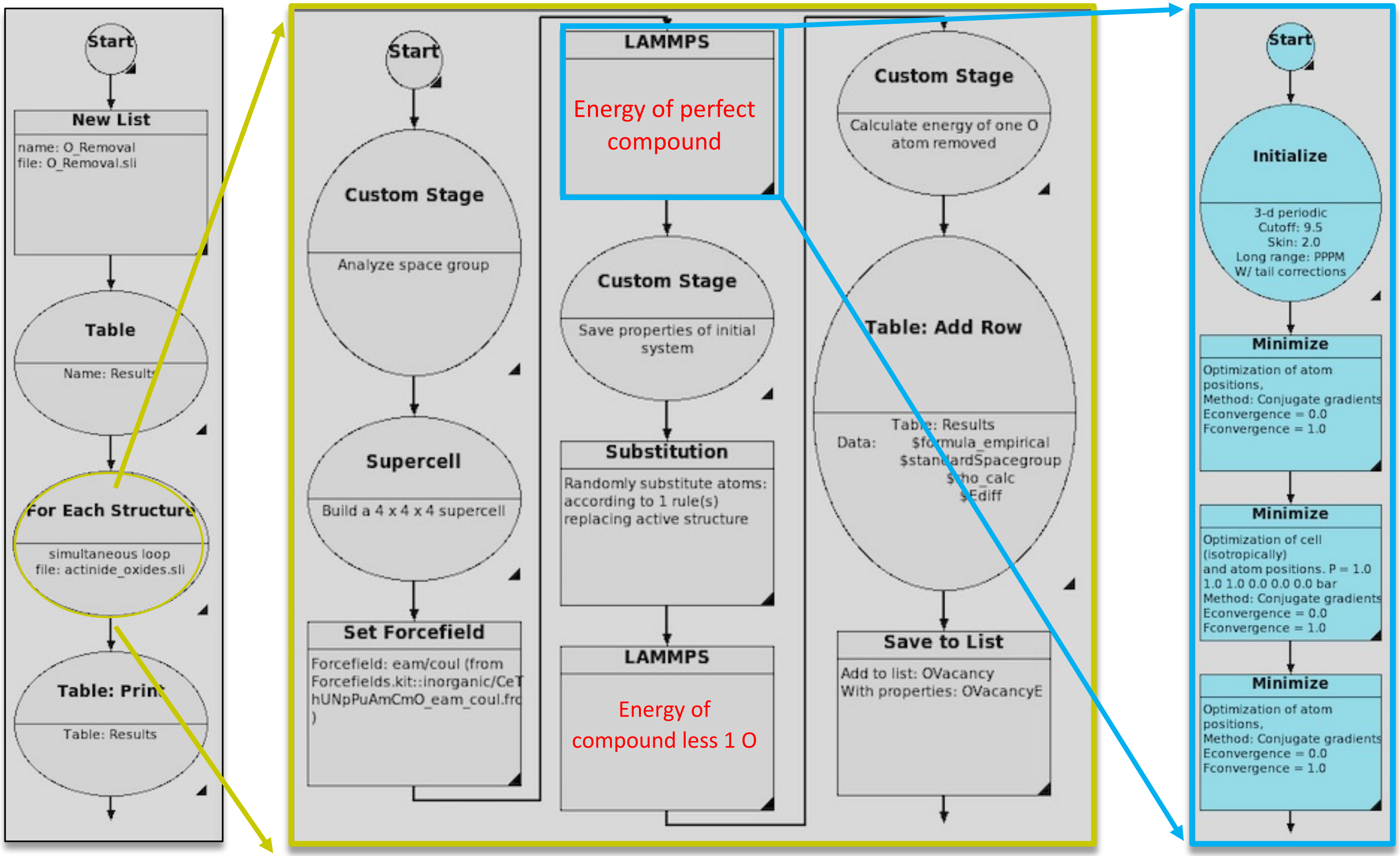
Versatilité



Calculs Haut Débit : Robustesse et Versatilité - VASP

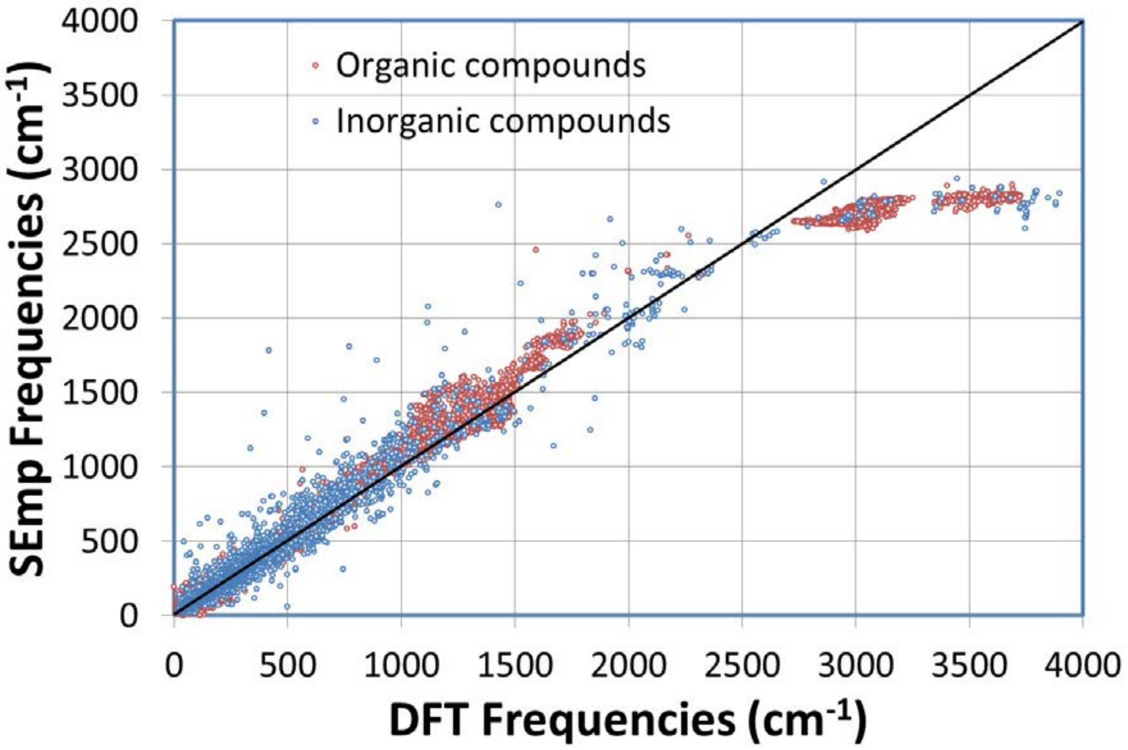


Calculs Haut Débit : Robustesse et Versatilité - LAMMPS



Calculs Haut Débit: Robustesse et Versatilité – GAUSSIAN et MOPAC

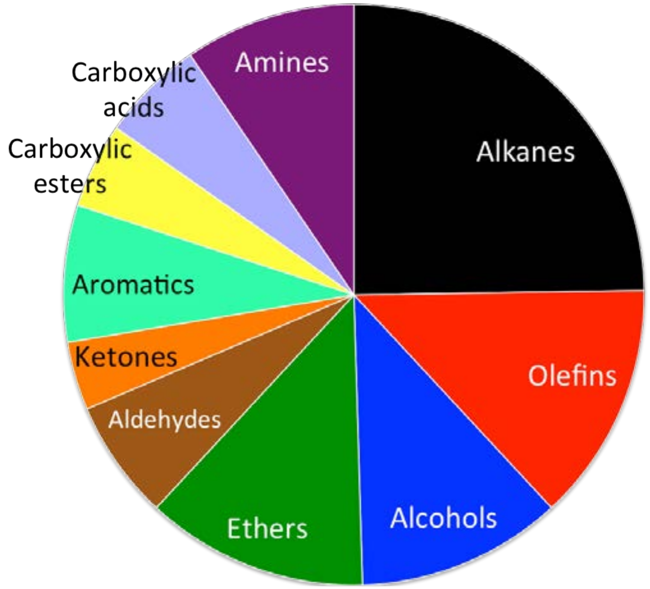
- Comparison between the vibrational frequencies computed with semi-empirical and DFT methods for organic and inorganic molecules: 1395 molecules, ~42,000 frequencies

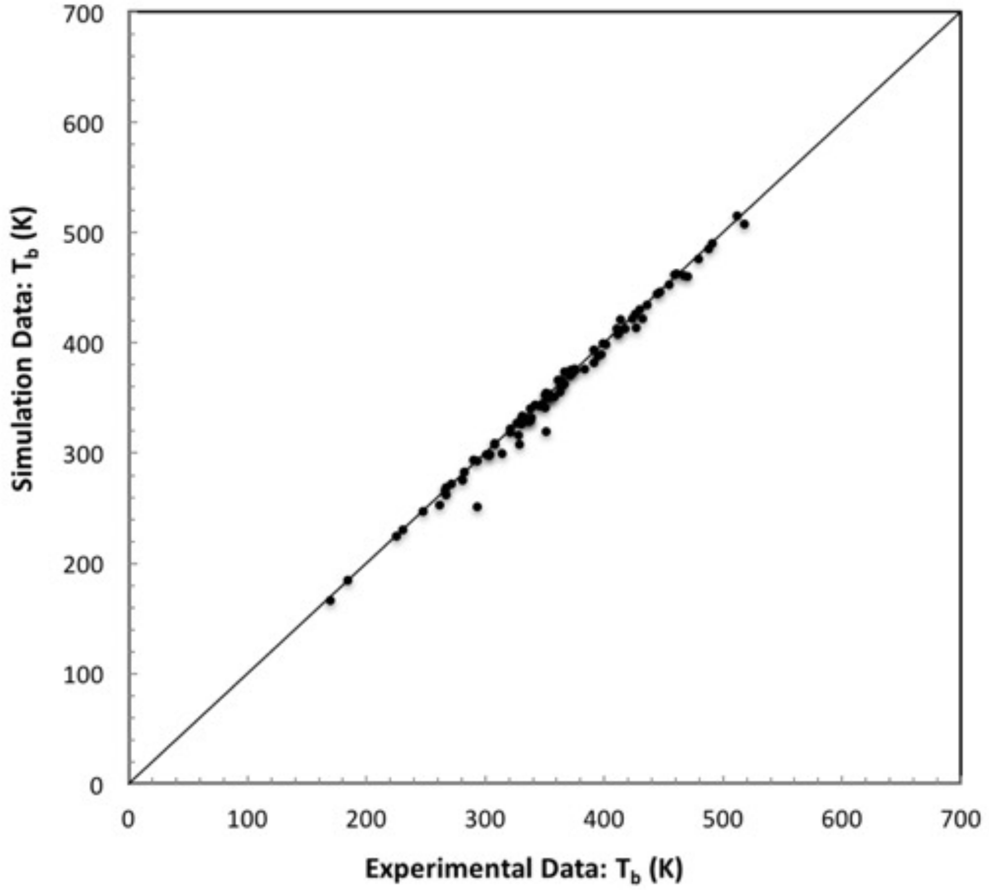


Rozanska *et al. J. Chem. Eng. Data* **2014**, *59*, 3136-3143 & *Oil Gas Sci. Tech*. **2015**, 70, 405-417

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%

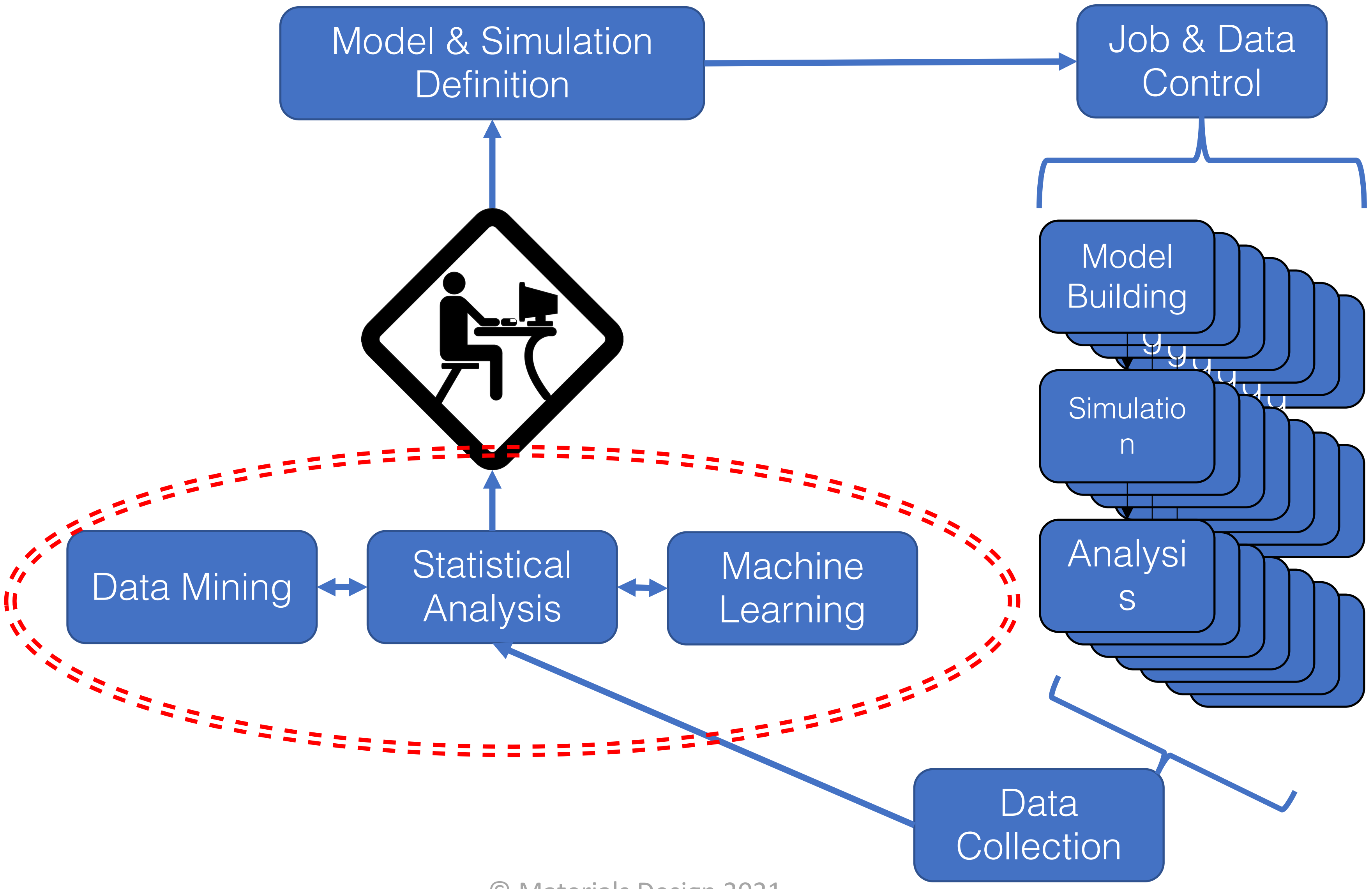




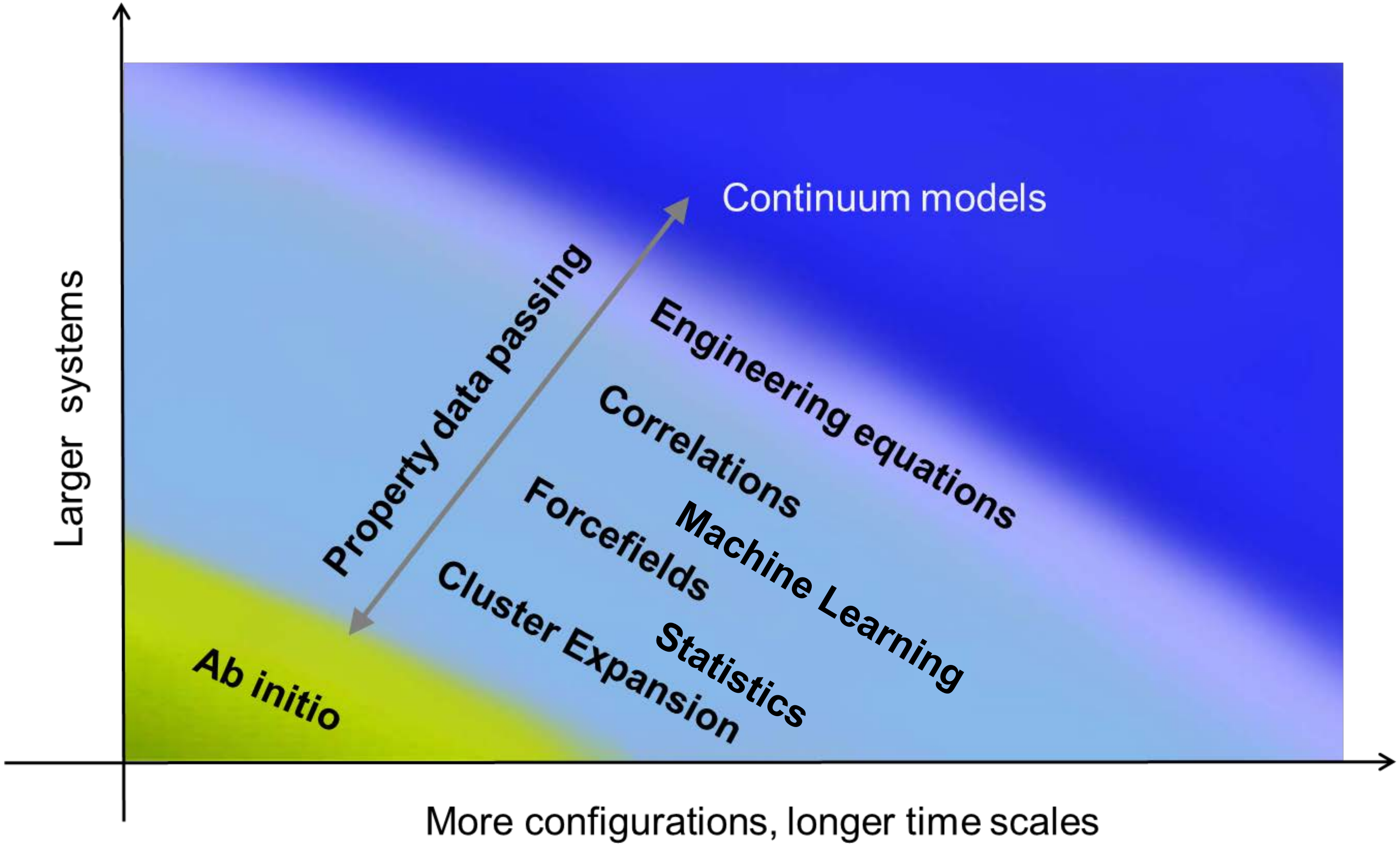
MedeA-GIBBS simulations (AUA & TraPPE-UA FF)

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

Analyse et Exploitation des Données



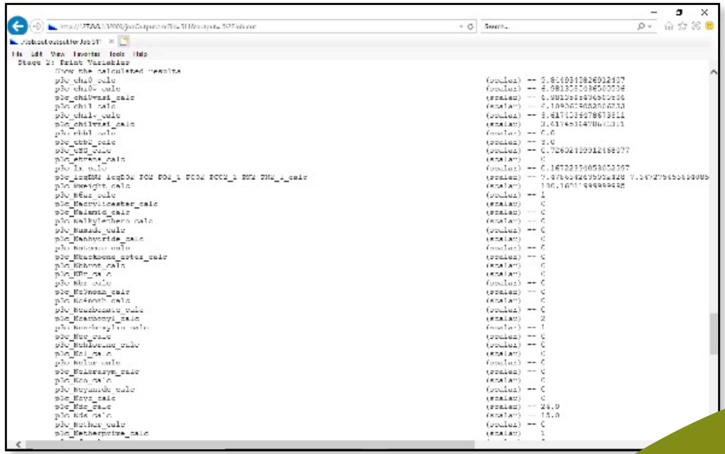
Liaisons entre propriétés et modèles par changement d'échelles de temps et de taille

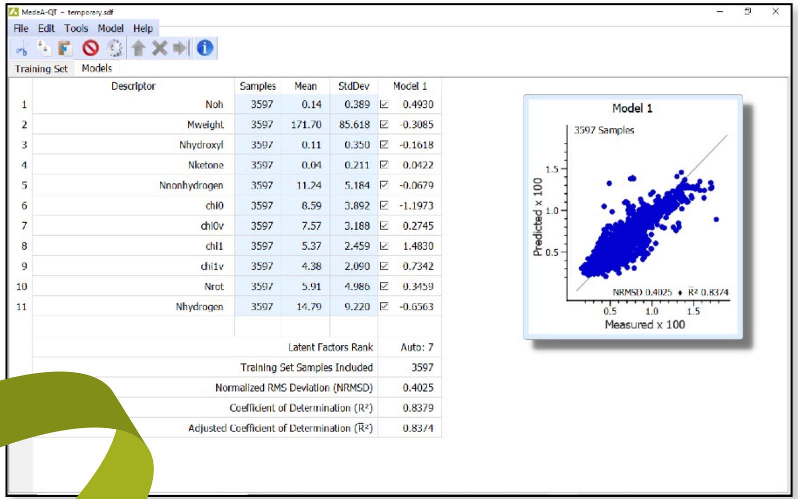


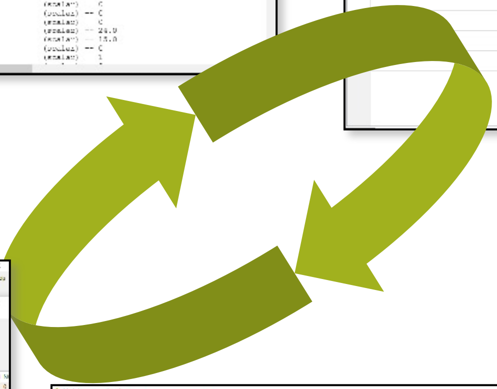
Analyse Statistique et Corrélation

MedeA QT

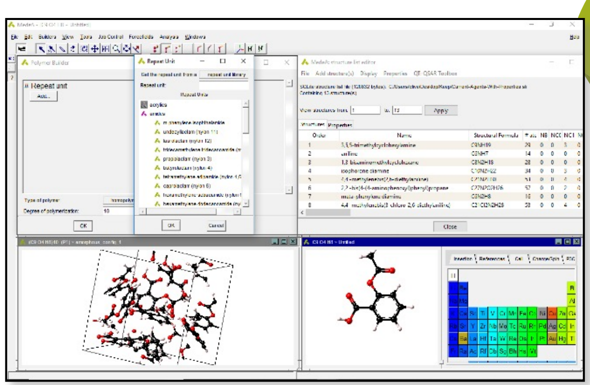
- *MedeA QT*
  PLS & MLR
- ML and integration



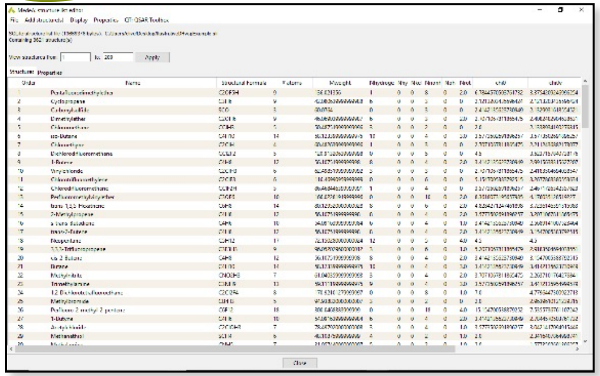




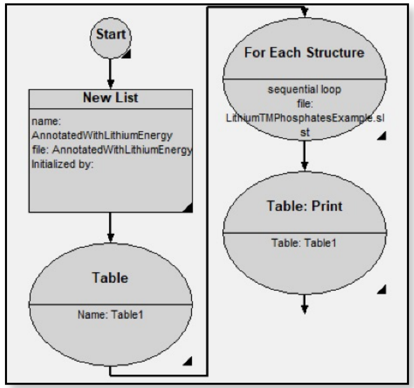
Flowchart based descriptors – chemistry simulation engine based, & proprietary



Creating molecules and systems using MedeA



Structure list - storing information

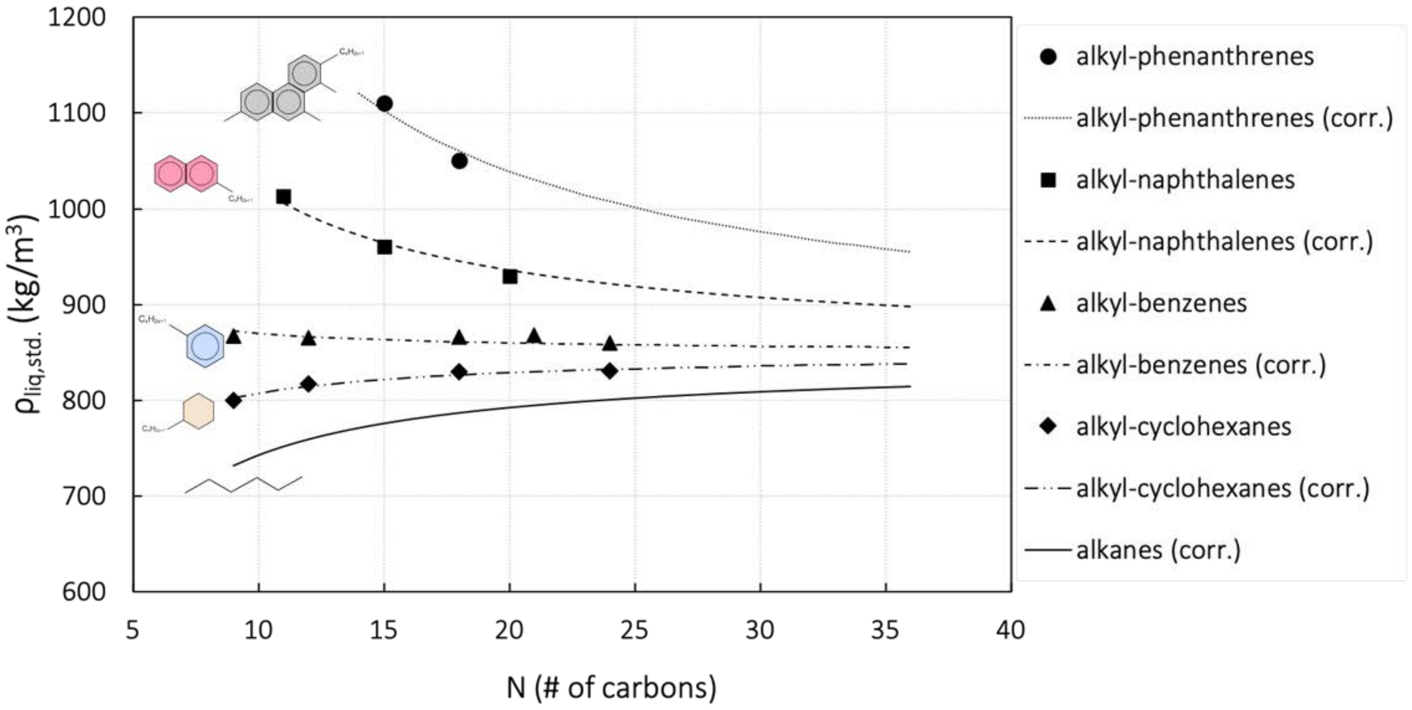


Flowchart based model usage

Modèles de Corrélation

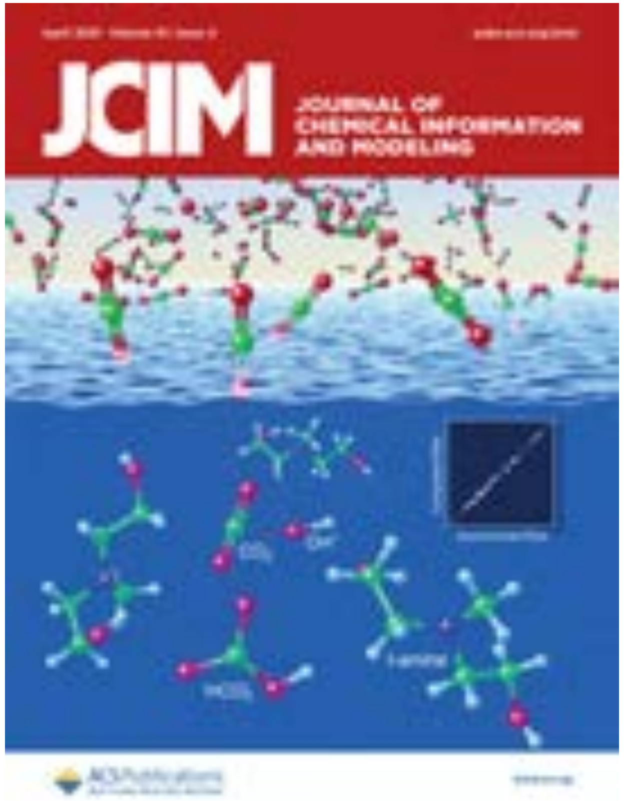
Use correlations to predict properties for other members of a chemical family

Heavy Crude Oil Components
Liquid Density Prediction



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

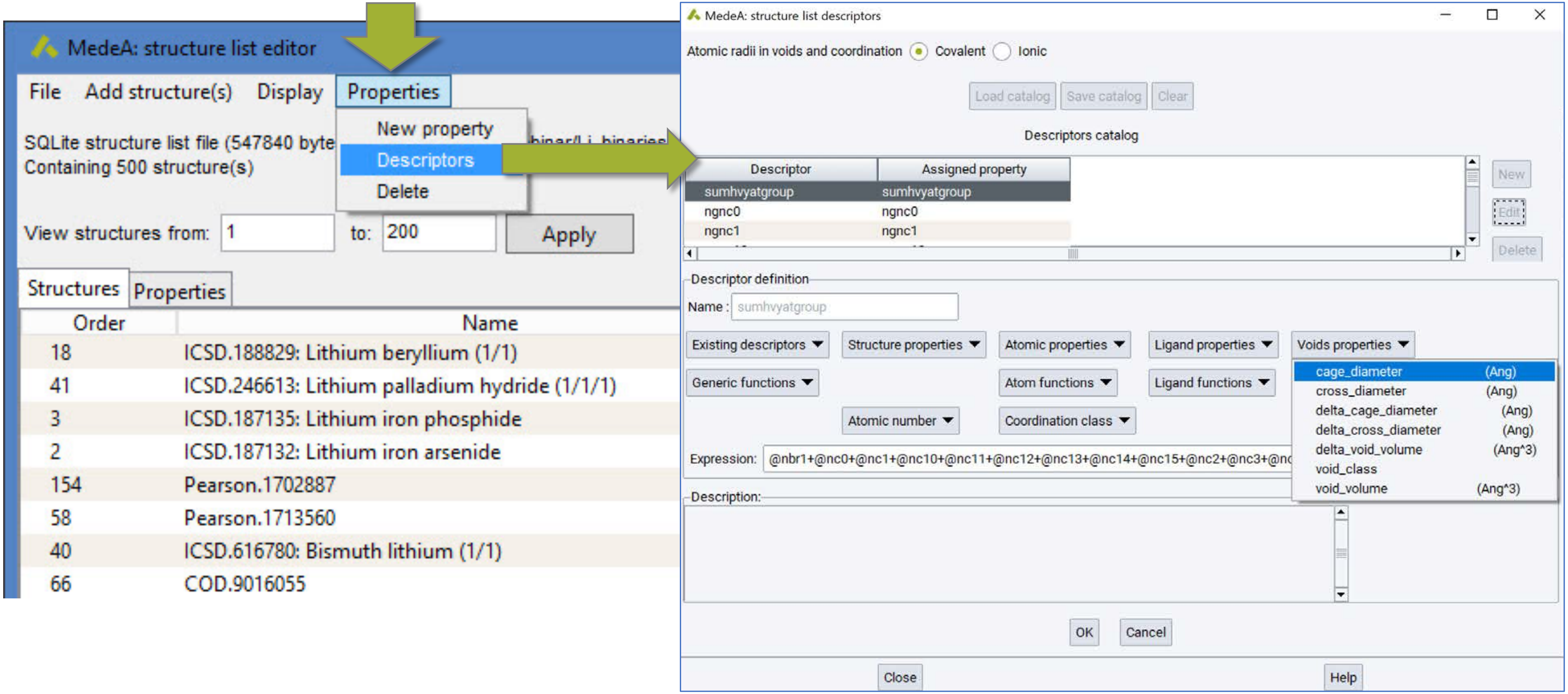
CO_2 Absorption Kinetics



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

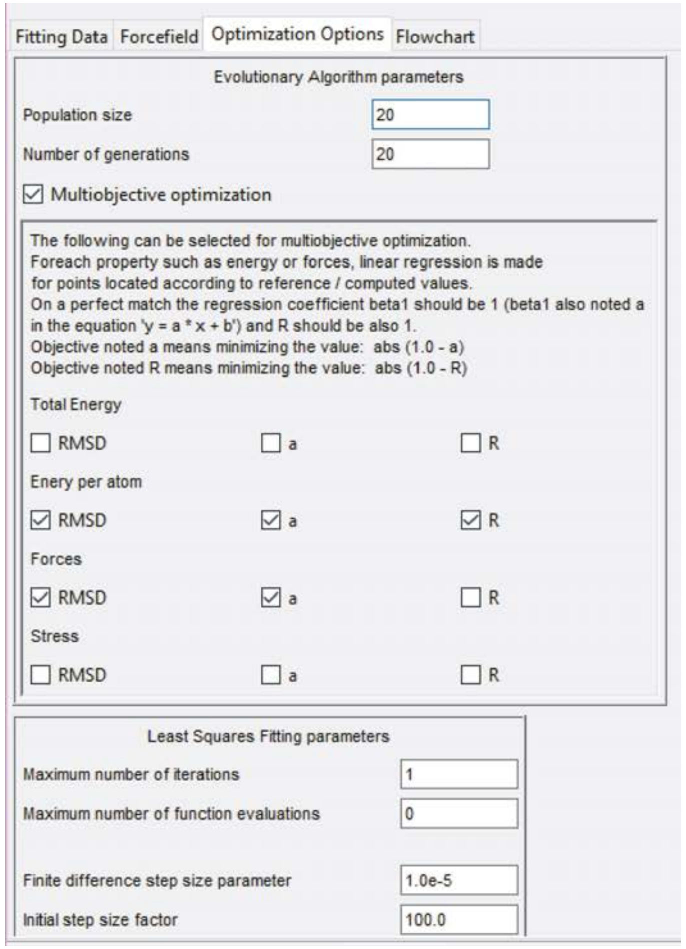
Éditeur de Liste de Structures : Propriétés et Descripteurs

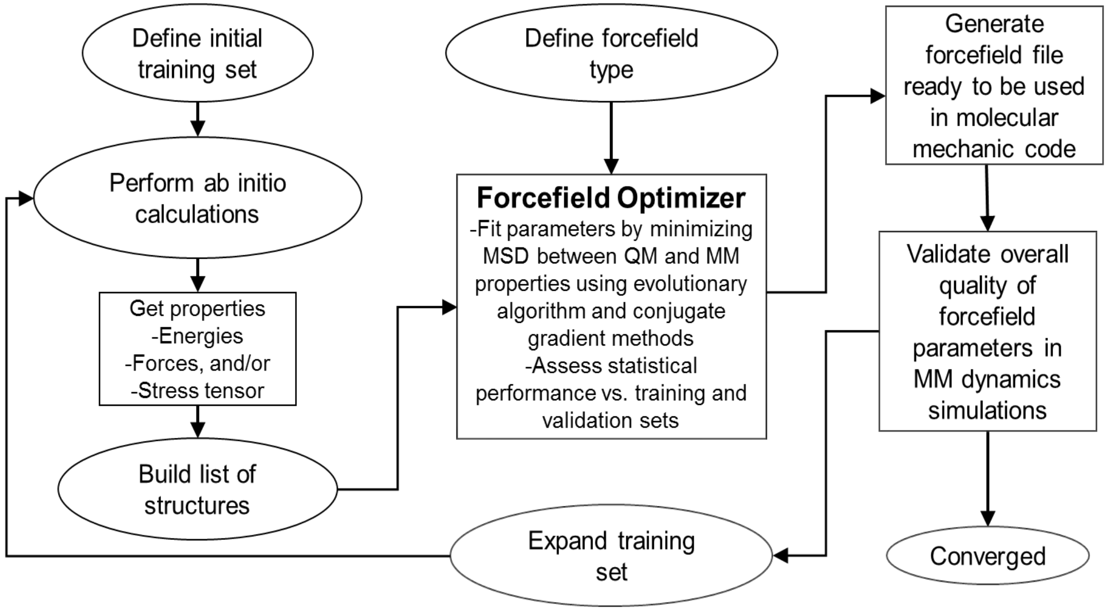
- *MedeA* offers a consistent basis for the construction of descriptors and correlations

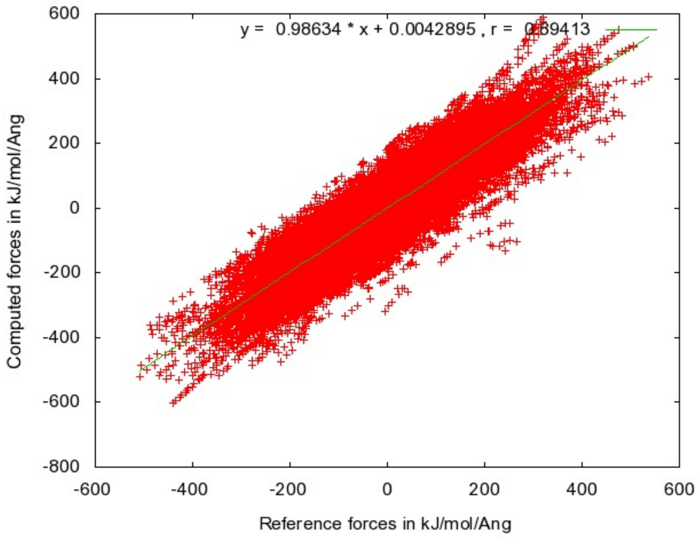


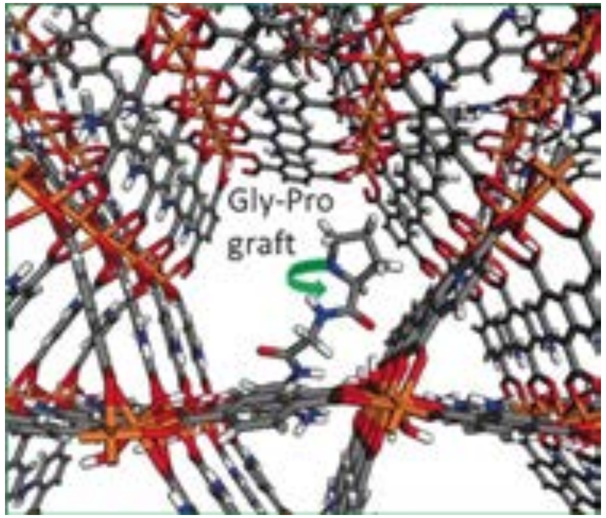
Optimisation de Paramètres de Champs de Forces par Algorithme d'Évolution Génétique

MedeA Forcefield Optimizer







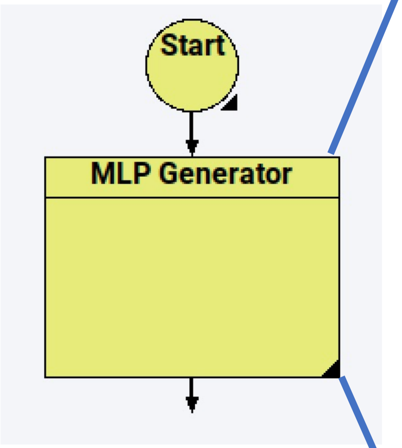


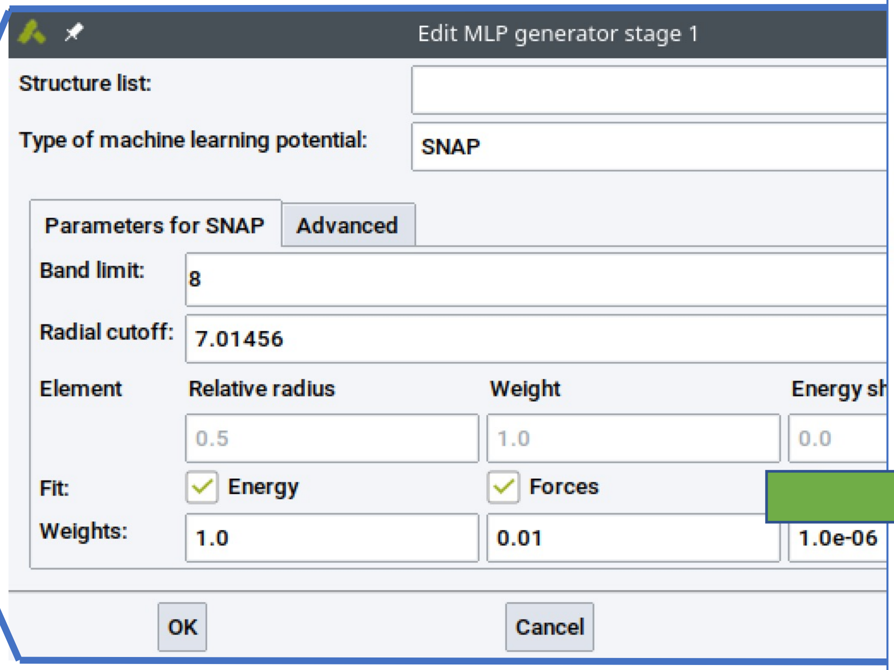
Todorova et al. *Chem. Eur. J.*, **2016**, *22*, 16531-16538.

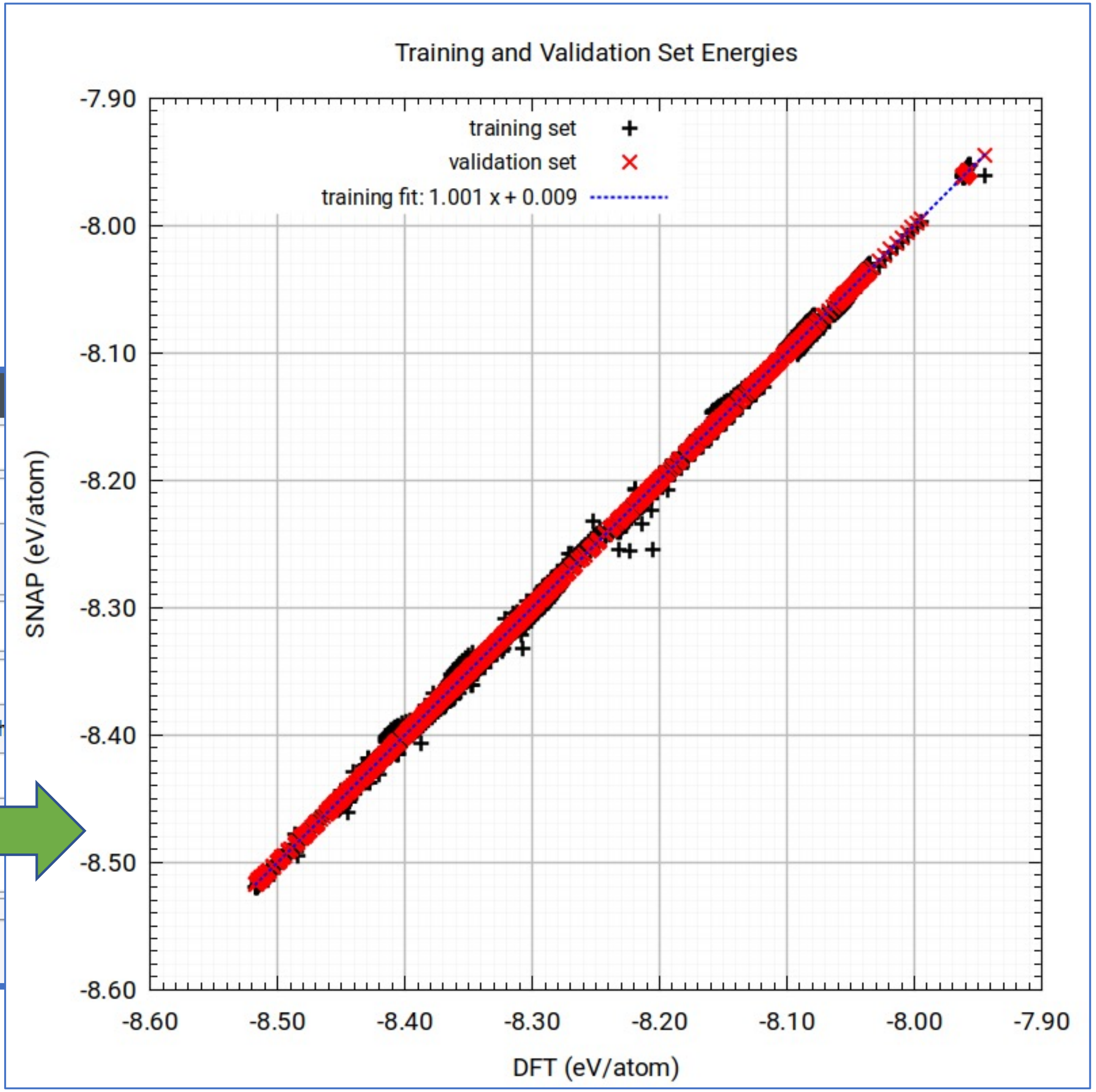
Optimisation de Champs de Forces par Méthode d'Auto-Apprentissage

MedeA MLP Generator

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

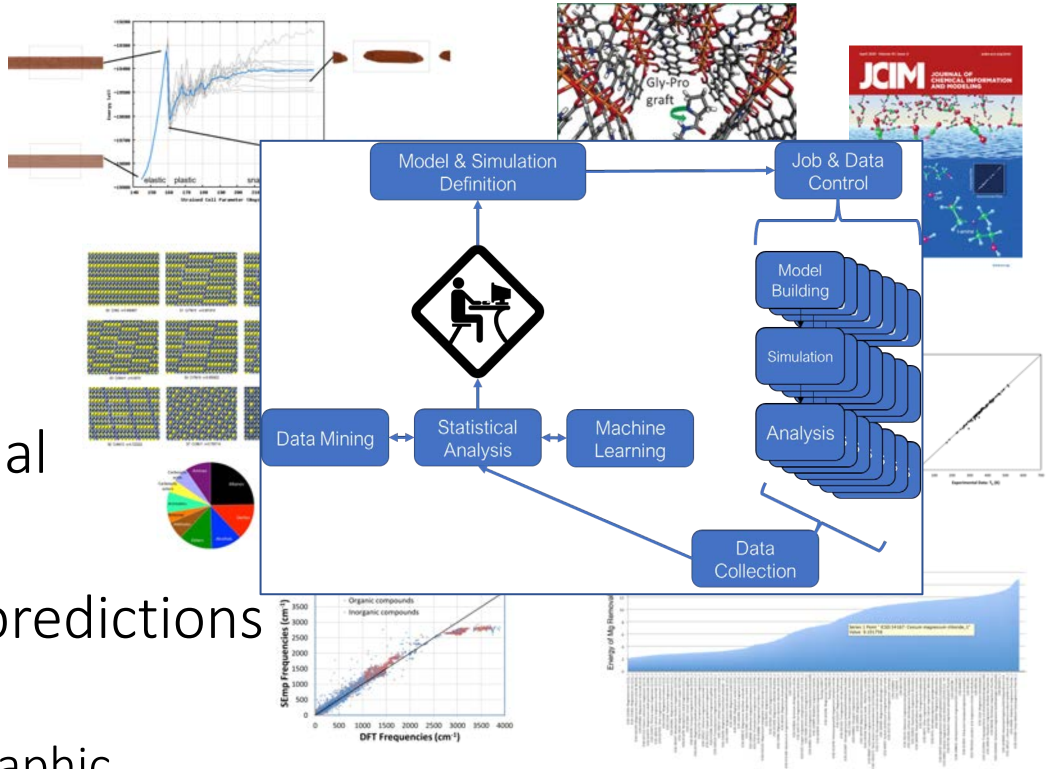






Résumé et Derniers Mots

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

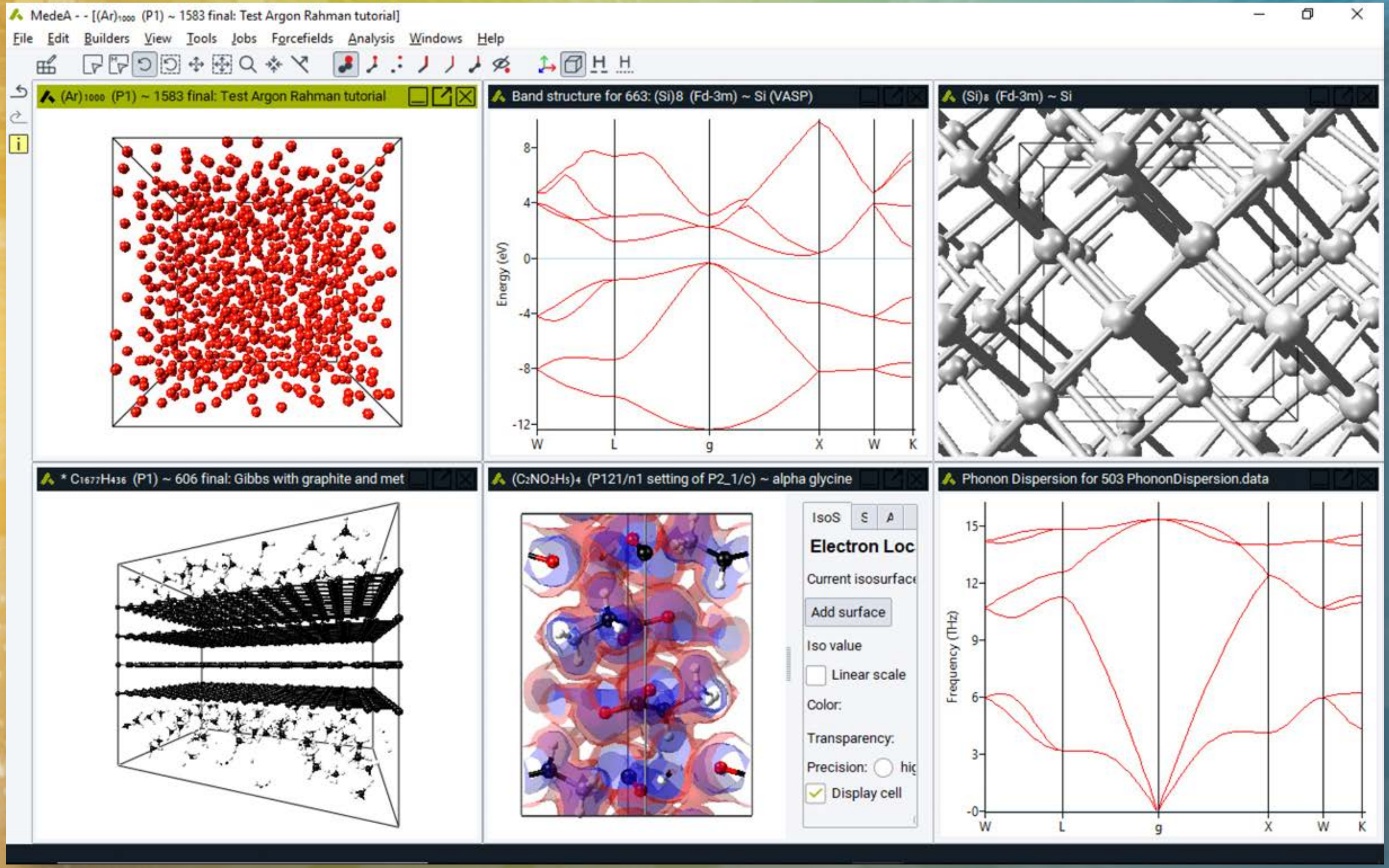
Materials Design

MedeA 3.3

Software Release

July 2021

www.materialsdesign.com/software-releases



Session de Questions et Réponses

Dr. Xavier Rozanska

Materials Design

Dr. Benoit Minisini

Materials Design

Pour toutes autres questions sur nos webinaires passés et futurs

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www.materialsdesign.com

MedeA

Innovation by Simulation