A Genomic Approach to Study the Properties and Correlations of MAX Phases

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I. Outline

I. Introduction to MAX phases

II. **Genomic** approach to study MAX phases

III. Computational methods

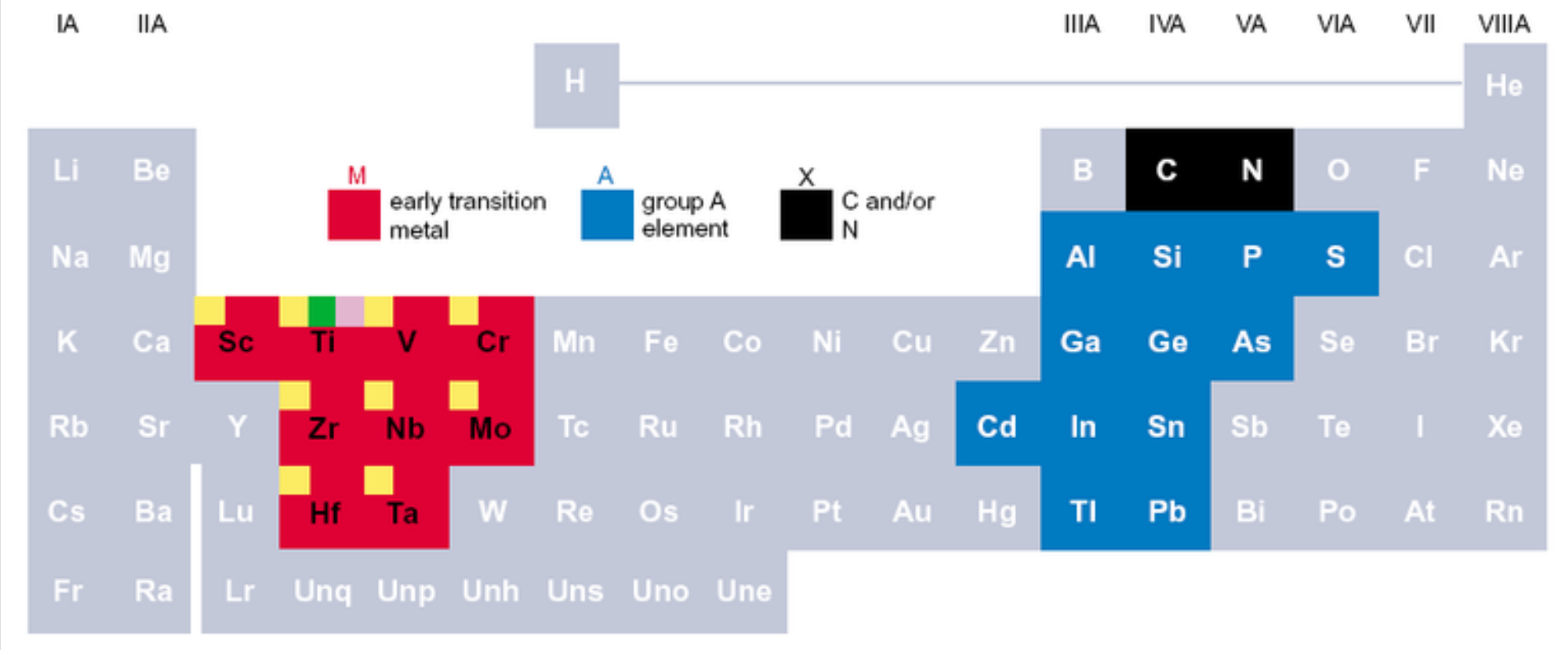
IV. Analysis of results

V. Summary and Conclusions

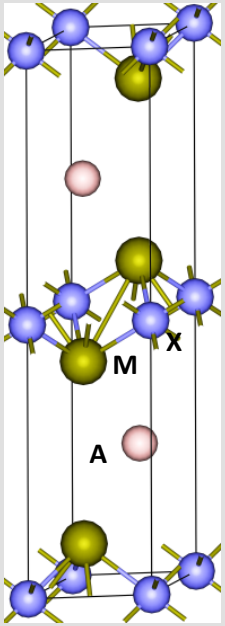
VI. Future work

I. Introduction to MAX Phases

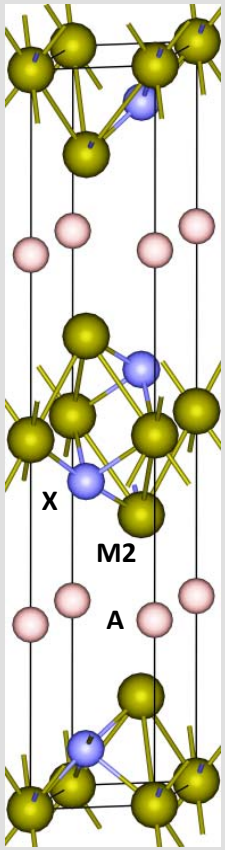
Why MAX phases? A novel class of intermetallic compounds with unique properties serving as a **model system** for **Genomic data base**.
What is MAX? Layered Ternary Transition Metal Carbides and Nitrides.
Formula: $M_{n+1}AX_n$ where **M** — Early Transition **M**etal; **A** — **A**-group element; **X** — Carbide or Nitride, *n* = 1,2,3,4. (*n* > 4 also possible)
Most MAX phases are 211 or 312 compounds; 413 and 514 are very rare.



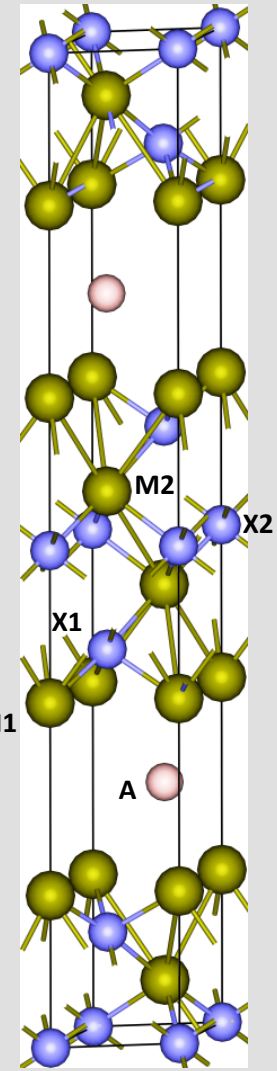
Sketch of layered hexagonal crystal structure of 211, 312, 413, 514 MAX phases



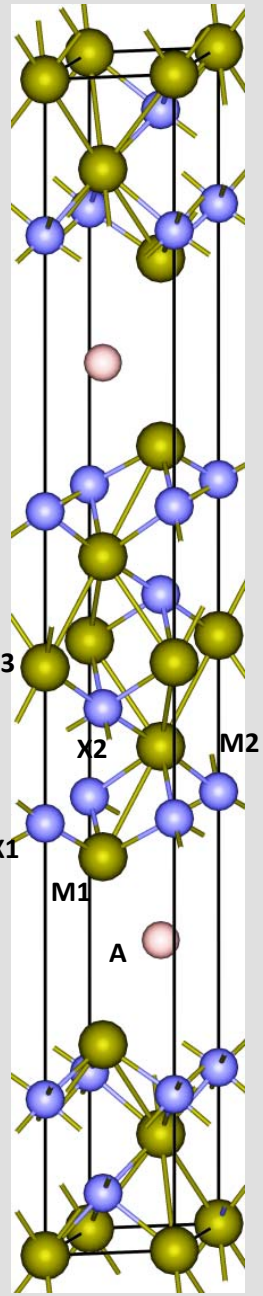
M_2AX



M_3AX_2



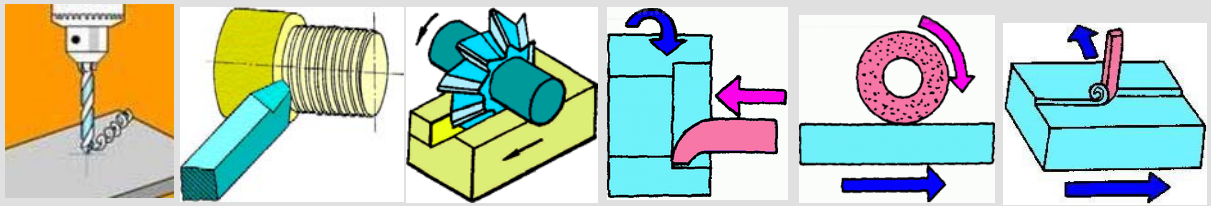
M_4AX_3



M_5AX_4

Special properties of MAX phases

♠ ***Like a Metal:*** thermally and electrically conductive, thermal-shock resistant, machinable, and damage tolerant;



Images from the Internet

♠ ***Like Ceramics:*** light weight, stiff, refractory and oxidation resistant, not expensive.

♠ **Mechanical properties of MAX phases are very complicated, depending on structure, composition and interatomic bonding.**

♠ **There are many real and projected applications for MAX phases.**

♠ **We focus on fundamental understanding and construction of the data base that can lead to these application.**

♠ **We explore its application to fossil energy technology.**

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II. Genomic approach to mechanical properties

- ♠ There are many published papers on properties of MAX phases but data are scattered.
- ♠ An ambitious approach: get data for **All MAX phases**, properly screened and studied in detail => a **genomic approach**.
- ♠ Construction of a "complete" data base for All possible MAX phases for statistical data-mining and machine learning.
- ♠ Consider trends in the rows and columns of elements **M**, and **A**.
- ♠ Consider difference between **X** = C and **X** = N and trends in n.
- ♠ Consider correlations between **M**, **A**, **X**.
- ♠ Consider connections to electronic structures and bonding.
- ♠ Predict new stable MAX phases having outstanding properties.
- ♠ Identify the **genes** in MAX phases for targeted applications.
- ♠ Focus on fundamental understanding of MAX phases compounds.

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III. Computational methods (DFT-based calculations)

Mechanical properties calculations:

Use Vienna *Ab initio* Simulation Package (**VASP**) for relaxation, a stress- strain analysis under linear elastic theory to first obtain elastic coefficients C_{ij}. Apply RVH approximation for poly-crystals to obtain bulk modulus (K), Shear modulus (G), Young's modulus (E) and Poisson's ratio (η), Pugh ratio G/K.

Electronic structure characterization:

Use first-principles orthogonalized linear combination of atomic orbitals (**OLCAO**) method for electronic structure calculation. OLCAO is a Density Functional Theory using LDA and atomic orbitals for basis expansion developed by us.

Effective Charge Q* on each atom, **Bond Order values** $\rho_{\alpha\beta}$ for each pair of atoms:

$$Q_\alpha^* = \sum_i \sum_{n,occ.} \sum_{j,\beta} C_{i\alpha}^{m^*} C_{j\beta}^{m} \langle b_{i\alpha}(\vec{k},\vec{r}) | b_{j\beta}(\vec{k},\vec{r}) \rangle$$

$$\rho_{\alpha\beta} = \sum_{n,occ.} \sum_{j,\beta} C_{i\alpha}^{n^*} C_{j\beta}^{n} \langle b_{i\alpha}(\vec{k},\vec{r}) | b_{j\beta}(\vec{k},\vec{r}) \rangle$$

We advocate that the **total bond order density** or **TBOD** (sum of all bonds in the crystal divided by volume) as the single most important parameter representing the electronic structures, the **gene**!

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Project started 1/1/2011. Papers published, accepted or submitted:

♠ Yuxiang Mo, Paul Rulis, **W.Y. Ching**, "Electronic Structure and Optical Conductivities of 20 MAX-Phase Compounds", Phys. Rev. B86, 165122-1-10 (2012).

♠ A. Misra and **W.Y. Ching**. "*Ab initio* multi-axial tensile stress-strain-failure behavior of crystalline hydroxyapatite". Scientific Research, #:1488 (2013).

♠ S. Aryal, M. C. Gao, L. Ouyang, and P. Rulis, **W. Y Ching,"***Ab initio* studies of Mo-based alloys: mechanical, elastic and vibrational properties", Intermetallics. 38, 116-125 (2013)

♠ **W.Y. Ching,** Yuxiang Mo, Sitaram Aryal and Paul Rulis, "Intrinsic mechanical properties of 20 MAX phase compounds", J. Amer. Ceram. Soc. 1-6 (2013).

♠ C. C. Dharamawardhana, R. Sakidja and **W. Y. Ching**, "Temperature dependent mechanical properties of Mo-Si-B compounds via ab-initio molecular dynamics", APL-Materials.1,012106 (2013).

♠. Liaoyuan Wang, Paul Rulis, **W. Y. Ching**, "Calculation of core-level excitation in some MAX phase compounds", J. Appl. Phys. 114, 023708 (2013).

♠. Neng Li, C. C. Dharamawardhana, K.L. Yao and **W.Y. Ching**, "Theoretical characterization on intrinsic ferromagnetic phase in naoscale laminated Cr_2GeC". Solid State Commun.,174 43–45 (2013).

♠. Neng Li, R. Sakidja and **W.Y. Ching,** "Oxidation of Cr2AlC (0001): "Insights from *ab initio* calculations", JOM, Published on line (2013). DOI: 10.1007/s11837-013-0741-x.

♠ Yuxiang Mo, S. Aryal, Paul Rulis and **W.Y. Ching**, "Crystalline Structure and Elastic properties of MAX-like $(Cr_2Hf)2AlC$", J. Amer. Ceram. Soc. (accepted and in press).

♠ Neng Li, R. Sakidja and **W.Y. Ching,** "DFT Characterization on the Oxidation Processes of a Single O Atom and O_2 Molecule on the Cr_2AlC (0001) Surface", submitted to Appl. Surface Sci.

♠ S. Aryal, Ridwan Sakidja, M. Barsoum and **W.Y. Ching**, "**A Genomic Approach to the Stability, Elastic and Electronic Properties of the MAX Phases", Physica Status Solidi B. (in Press)**

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Several more papers currently under preparation, expect to be published this year.

♠ A. Hussain, R. Sakidja, and W-Y Ching, *Ab initio* Molecular Dynamics (AIMD) Study and Potential Development of Ti-Si-C Metallic System, to be submitted

♠ R. Sakidja and W-Y Ching, Ab Initio Molecular Dynamics (AIMD) Study on Phase Stability and Li Ion Mobility on 2-D MXenes (M = Group IVB – VIB, X = C/N), to be submitted.

♠ . C.C. Dharmawardhana, R. Sakidja, S. Aryal, W. Y. Ching, Computational design of thermal expansion in Mo_5Si_3 - T1 alloyed phase, to be submitted.

♠ R. Sakidja, N. Li and W-Y Ching, Ab initio Molecular Dynamics (AIMD) Study on the Early Stage of Oxidation on Cr_2AlC and Ti_2AlC MAX Phases, in preparation

♠ R. Sakidja and A. Hussain and W-Y Ching, Development of Embedded Atom Model (EAM) and Angular Dependent Potential (ADP) for Ti-Al-C Ternary System, in preparation.

♠ C Dahkal, S. Aryal, R. Sakidja, and W. Y. Ching, In what way MAX nitrides differ from MAX carbides and why? in preparation.

IV. Analysis of results MAX phases

Phase I: Test calculations on 20 MAX phases. (first 2 years!)

♠ Select **20** MAX phases of different components and compositions.

♠ Calculate the electronic structure, bonding & optical conductivities of these 20 MAX phases. **(Done!)**

Yuxiang Mo, Paul Rulis, W.Y. Ching, "Electronic Structure and Optical Conductivities of 20 MAX-Phase Compounds", Phys. Rev. B86, 165122-1-10 (2012).

♠ Calculate the elastic and mechanical properties of the same 20 MAX phases. **(Done!)**

W.Y. Ching, Yuxiang Mo, Sitaram Aryal and Paul Rulis, "Intrinsic mechanical properties of 20 MAX phase compounds", J. Amer. Ceram. Soc. 1-6 (2013) DOI:10.111/jace.12376

♠ **Phases II**, all MAX phases! (This presentation!)

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Elastic coefficients and mechanical properties of 20 MAX phases

Crystals	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	K	G	E	η	G/K=k
Ti_3AlC_2	355.8	81.4	75.3	293.4	120.3	137.2	162.5	126.7	301.7	0.191	0.78
Ti_3SiC_2	369.6	96.2	107.6	358.3	155.0	136.7	191.1	141.3	340.0	0.204	0.74
Ti_3GeC_2	362.0	97.2	97.7	332.0	137.3	132.4	182.2	132.2	319.3	0.208	0.73
Ti_2AlC	301.9	68.0	63.0	267.9	105.1	117.0	139.7	110.5	262.3	0.187	0.79
Ti_2GaC	300.8	79.2	63.8	246.5	92.4	110.8	139.3	101.4	244.9	0.207	0.73
Ti_2InC	284.4	69.3	55.2	235.5	83.9	107.5	128.6	96.0	230.5	0.201	0.75
Ti_2SiC	312.9	82.1	110.4	329.2	149.6	115.4	173.0	124.9	302.0	0.209	0.72
Ti_2GeC	296.6	85.7	96.8	297.1	121.5	105.5	161.0	110.0	268.8	0.222	0.68
Ti_2SnC	262.6	88.6	73.1	255.2	96.8	87.0	138.8	92.4	226.8	0.228	0.67
Ti_2PC	**256.8**	144.8	155.0	**339.5**	166.3	56.0	191.8	93.1	240.4	**0.291**	**0.49**
Ti_2AsC	**212.9**	180.4	123.7	**289.5**	146.3	16.2	150.7	57.2	152.3	**0.332**	**0.38**
Ti_2SC	339.8	101.4	109.7	361.9	159.5	119.2	186.8	134.4	325.2	0.210	0.72
Ti_2AlN	312.9	73.0	95.5	290.7	126.1	120.0	160.5	117.4	283.1	0.206	0.73
V_2AlC	334.4	71.5	106.0	320.8	149.8	131.5	172.9	132.1	315.9	0.196	0.76
Nb_2AlC	316.6	86.3	117.0	288.6	137.6	115.2	173.6	116.4	285.5	0.226	0.67
Cr_2AlC	366.3	85.8	111.3	356.9	142.9	140.2	189.6	137.0	331.2	0.209	0.72
Ta_2AlC	344.5	112.2	137.1	327.9	152.3	116.1	198.8	124.1	308.1	0.242	0.62
α-Ta_3AlC_2	453.6	130.5	135.6	388.4	175.0	161.5	232.8	161.1	392.8	0.219	0.69
α-Ta_4AlC_3	459.2	149.1	148.7	383.1	170.5	155.0	243.0	155.3	384.1	0.237	0.64
Ta_5AlC_4	481.5	149.6	158.1	423.6	188.8	165.9	257.2	169.1	416.0	0.231	0.66

Anisotropic ratio C_{33}/C_{11} correlates with G/K. Note: Ti_2PC and Ti_2AsC are outliers.

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Electronic structure and bonding in the same 20 MAX phases

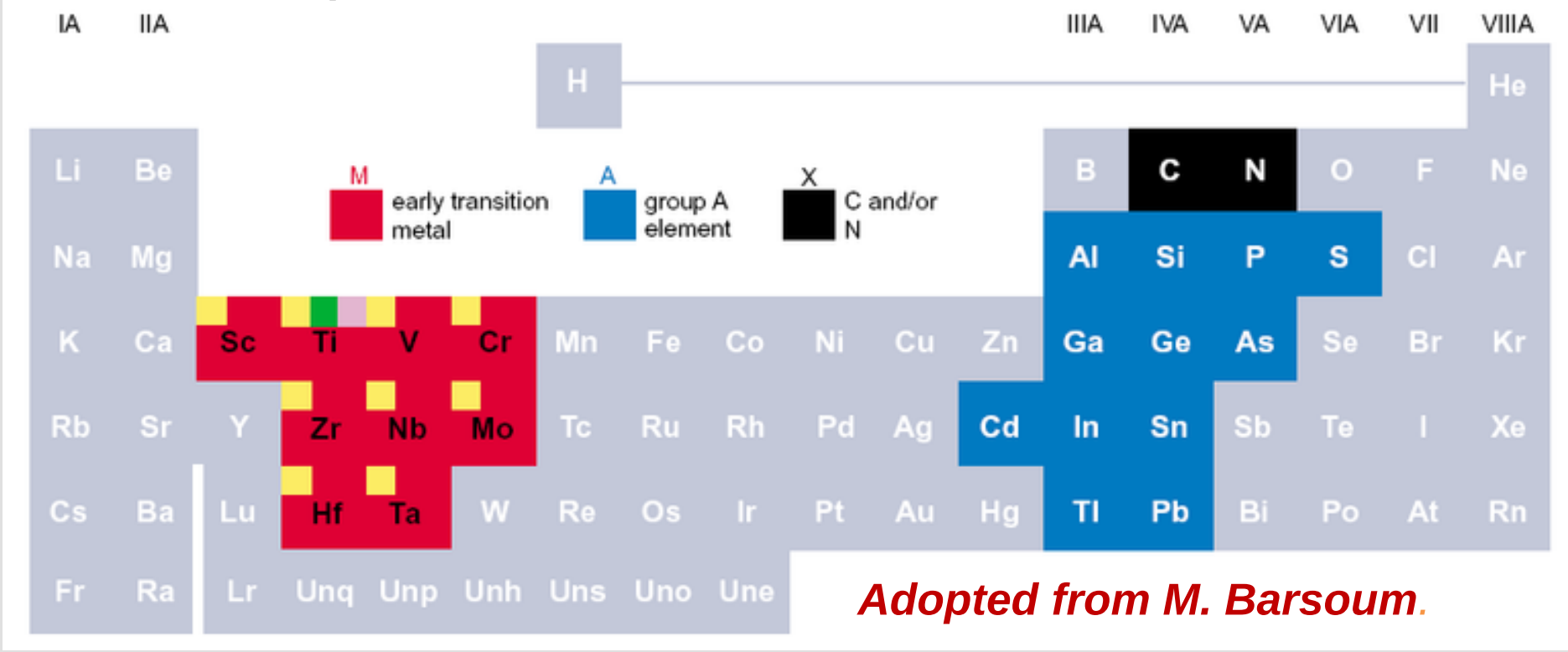
MAX	ΔQ*(M)	ΔQ*(X)	ΔQ*(A)	TBO	BO(M-X)	BO(M-M)	BO(M-A)	BO(A-A)	$N(E_F)$
Ti_2AlC	-0.330	-0.043	0.703	23.510	10.258	4.512	7.231	1.508	11.052
Ti_2GaC	-0.485	0.269	0.701	22.680	10.289	4.060	6.986	1.340	10.572
Ti_2InC	-0.424	0.148	0.700	22.750	10.238	4.396	6.482	1.636	9.260
Ti_2SiC	-0.393	0.097	0.688	22.820	10.344	3.583	8.153	0.742	12.921
Ti_2GeC	-0.509	0.324	0.694	21.750	10.337	3.541	7.111	0.758	14.720
Ti_2SnC	-0.381	0.069	0.693	22.320	10.294	3.926	7.110	0.993	15.084
Ti_2PC	-0.454	0.210	0.699	22.740	10.366	2.802	9.571	0.000	21.762
Ti_2AsC	-0.505	0.316	0.695	21.360	10.382	2.893	8.086	0.000	19.697
Ti_2SC	-0.447	0.189	0.705	21.340	10.380	2.944	8.018	0.000	7.301
Ti_2AlN	-0.295	-0.087	0.679	22.150	8.702	4.646	7.217	1.585	15.502
V_2AlC	-0.277	-0.101	0.655	22.820	10.017	4.192	6.905	1.704	21.663
Nb_2AlC	-0.493	0.245	0.741	15.410	7.319	1.253	5.354	1.399	13.338
Cr_2AlC	-0.098	-0.324	0.521	21.250	9.559	2.837	7.080	1.769	24.384
Ta_2AlC	-0.324	-0.044	0.692	24.810	10.130	5.724	7.561	1.397	11.126

We now have such data Table for **ALL** MAX phases.

Data publically available: Physica Status Solidi B. (in Press).

M (9): Sc (III_A);Ti, Zr, Hf (IV_A); V, Nb, Ta (V_A); Cr, Mo (VI_A).
A (11): Al, Ga, In, Tl (III_B); Si, Ge, Sn, Pb (IV_B); P, As (V_B); S(VI_B).
X (2): C (IV_B) or N (V_B).
n = 1, 211 phase; n = 2, 312 phase; n = 3, 413 phases; n = 4, 514 phase.

Possible MAX phase considered: 9 x 11 x 2 x 4 = 792!



Phase II: Expand to all 792 MAX phases. **(**This presentation!)

♠ Screen 792 MAX phases for mechanical (use Born Cauchy criterion) and thermodynamic stability (use heat of formation).

♠ Screening resulted in a large database of 665 viable MAX crystals.

♠ Find the **trends** and **correlations** in properties:

(1) Between elastic properties,

(2) Between electronic properties,

(3) Between mechanical and electronic structures.

♠ Only a few **selective results** on above properties and correlations are presented here due to time limitation.

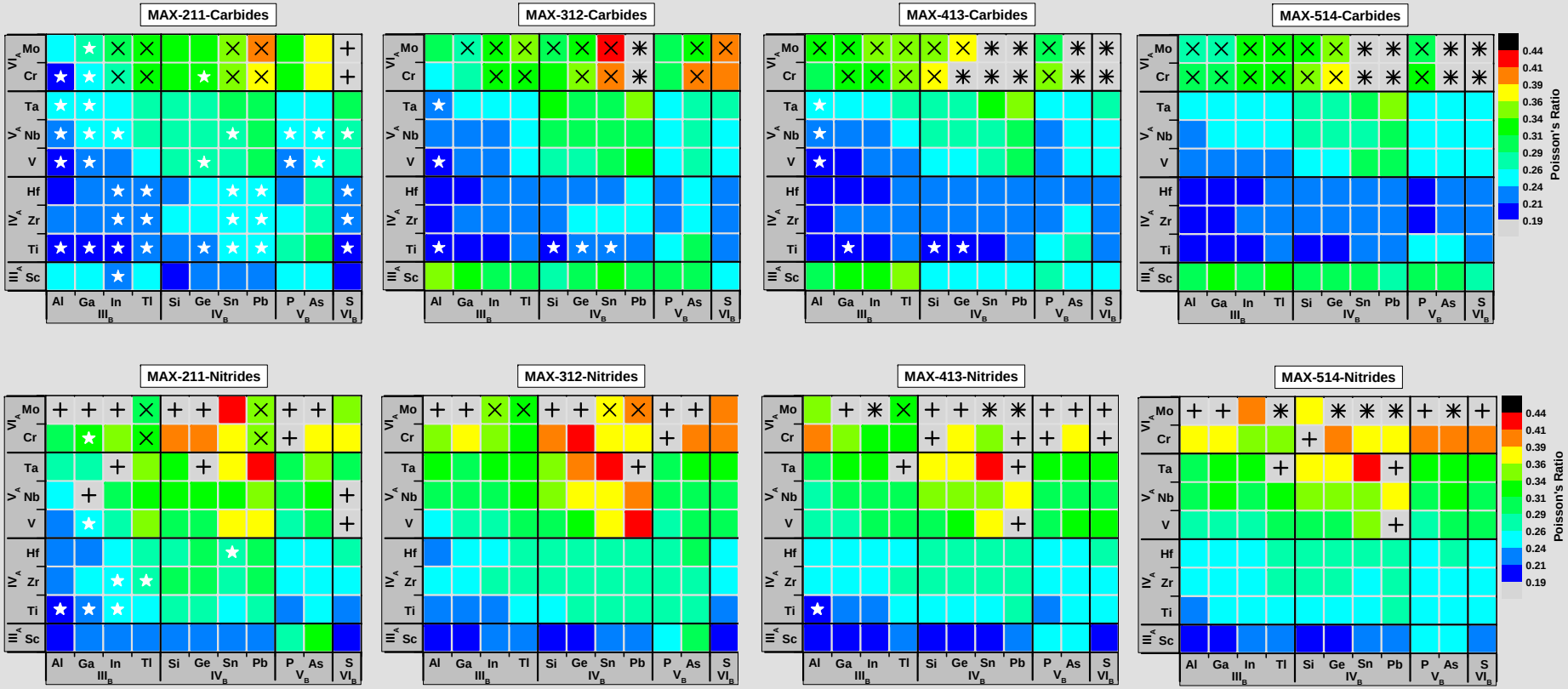
♠ Use the database to test efficacy of **data-mining algorithm**.

♠ Predict stable **new phases** (outliers) with special properties.

Warning! Results presented below are very selective & highly condensed!

792 unscreened data in the form of Maps.

665 screened data in the form of scattered plots.



♠ Poisson's ratio (η) maps for all MAX carbides (upper) and nitrides (lower) according to M (Y-axis) and A (X-axis) elements. Color in the box represents calculated η values.

♠ Stars in the box indicate => phases have been synthesized. '+' stands for elastic instability; '×' indicates thermodynamic instability (HoF).

♠ All confirmed MAX phases (~60 of them) are stable. There are more stable ones unexplored.

G/K, the most representative value for the mechanical properties. Data for 665 MAX phases passed the screen are presented!

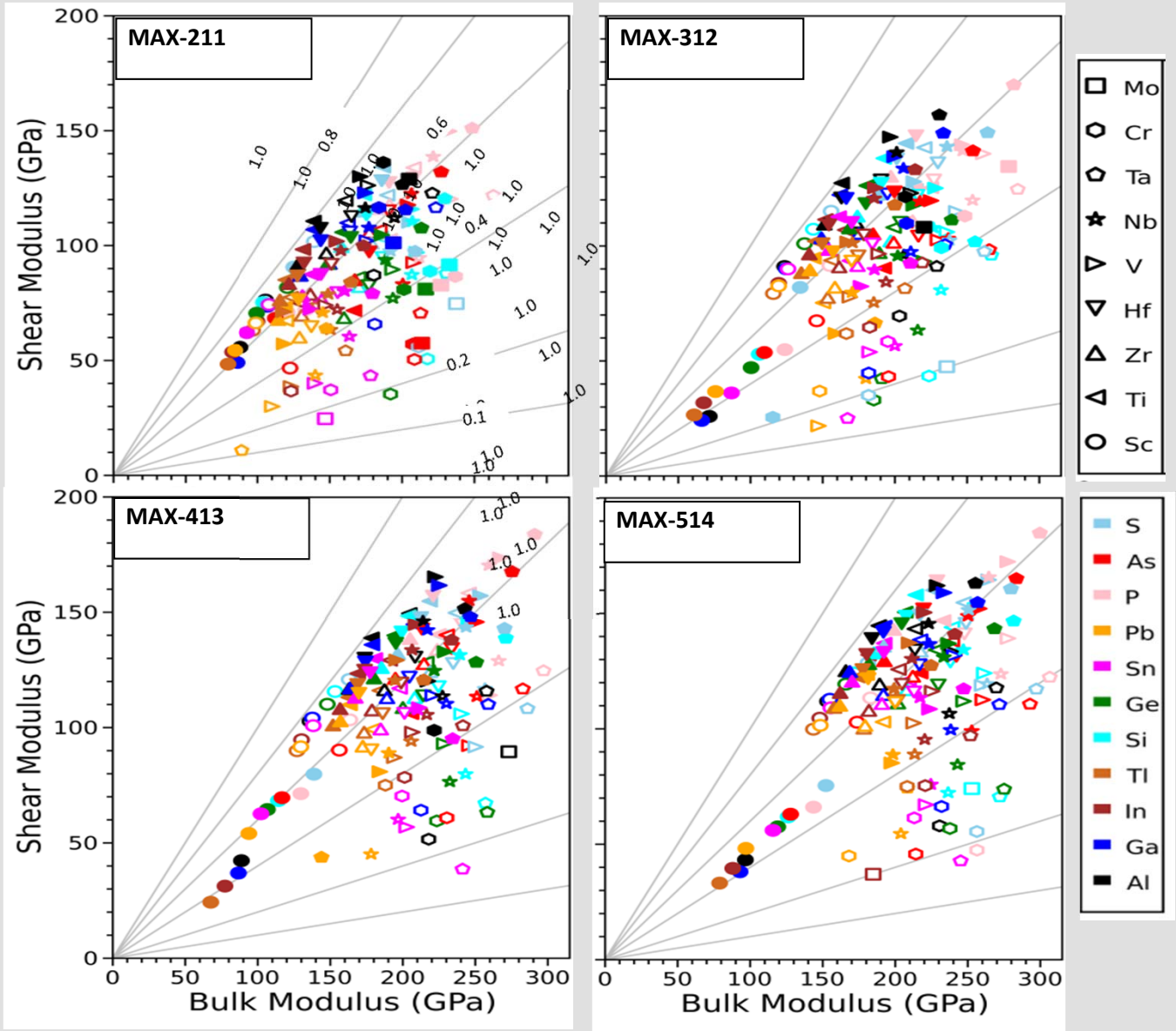
Comments:

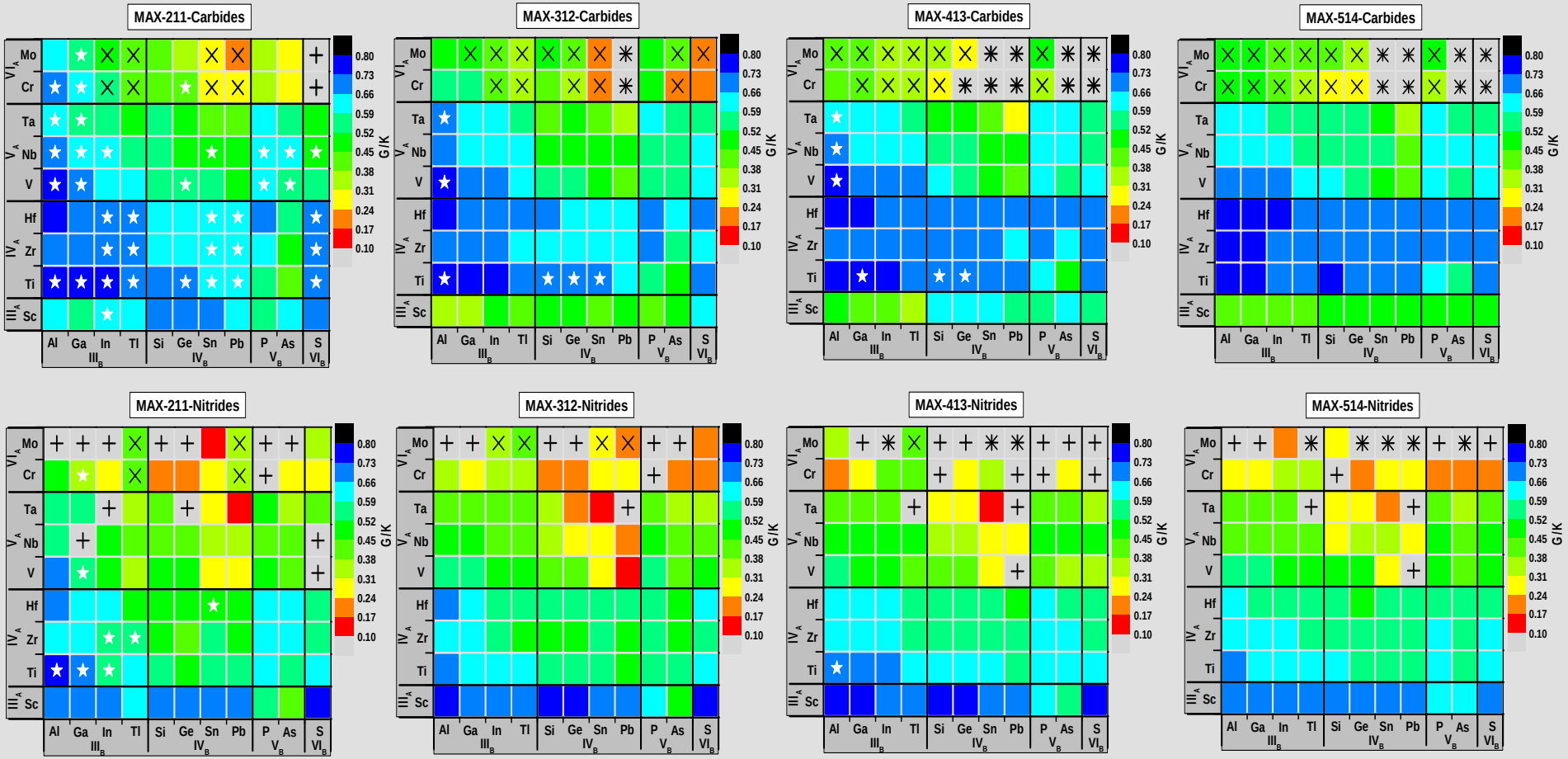
♠ Very busy slide: Different shape for different **M**, different color for different **A**.

♠ <u>All data</u> for G and K plotted on a single figure.

♠ Slopes give G/K ratio for each crystal!

♠ G/K map in the next slide.

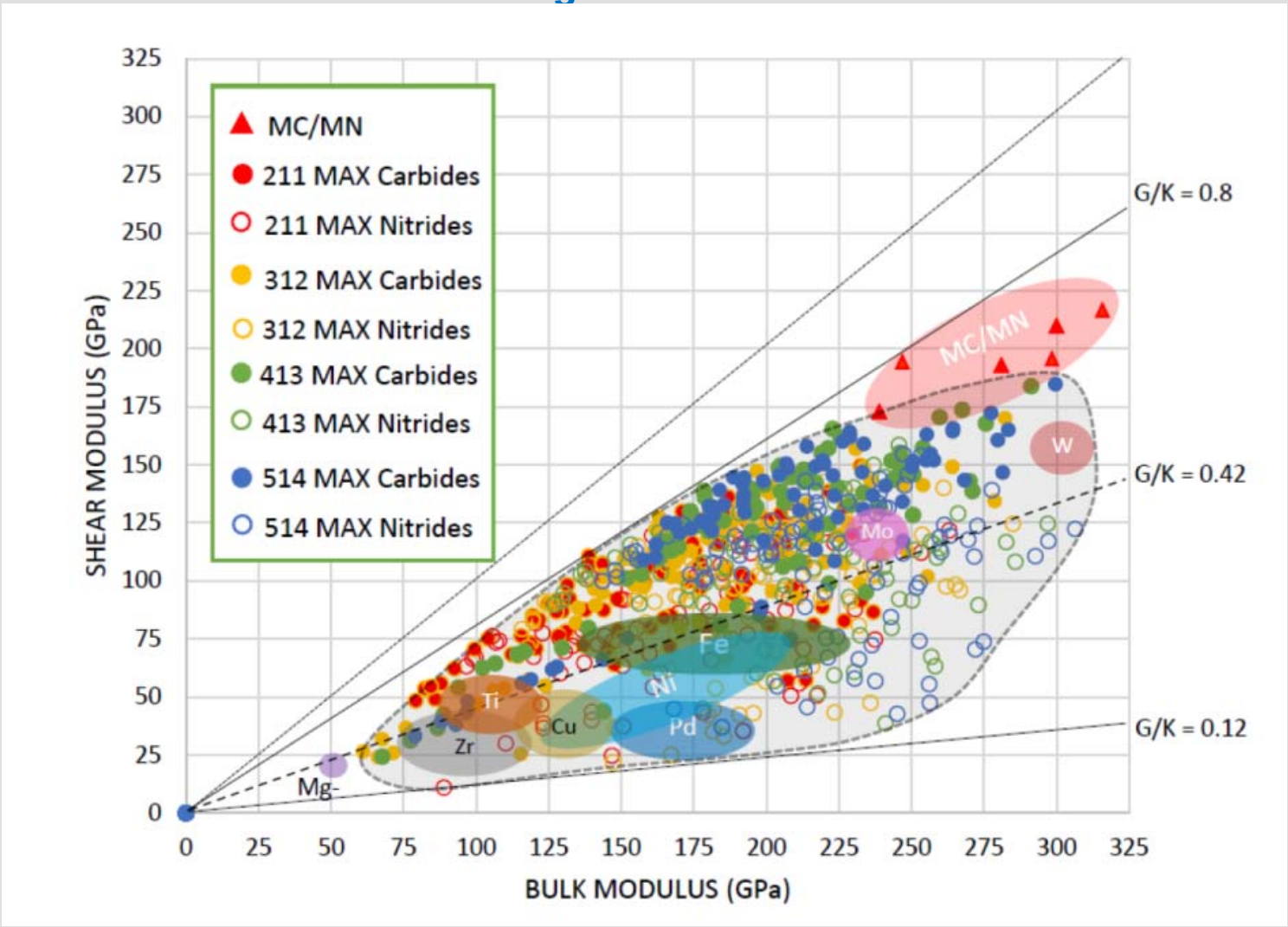




G/K maps for all MAX carbides (upper) and nitrides (lower) according to M (Y-axis) and A (X-axis) elements. Color in the box represents calculated G/K values. (This plot is similar to previous one for the Poisson's ratio.)

Bulk modulus K vs. Shear modulus G plot for all MAX phases

G/K = Pugh modulus ratio



MAX covers a wide range of G/K (0.8 – 0.18). Both ductile (G/K < 0.42) and brittle (G/K > 0.42).
Note the difference between nitrides and carbides.

(1) Elastic Property Results:

Correlation plots of linear elastic constants C_{11} vs C_{33} (left) and shear elastic constants C_{44} vs. C_{66} (right).

Comments:

♠ Data are very scattered depending on M,A,X.

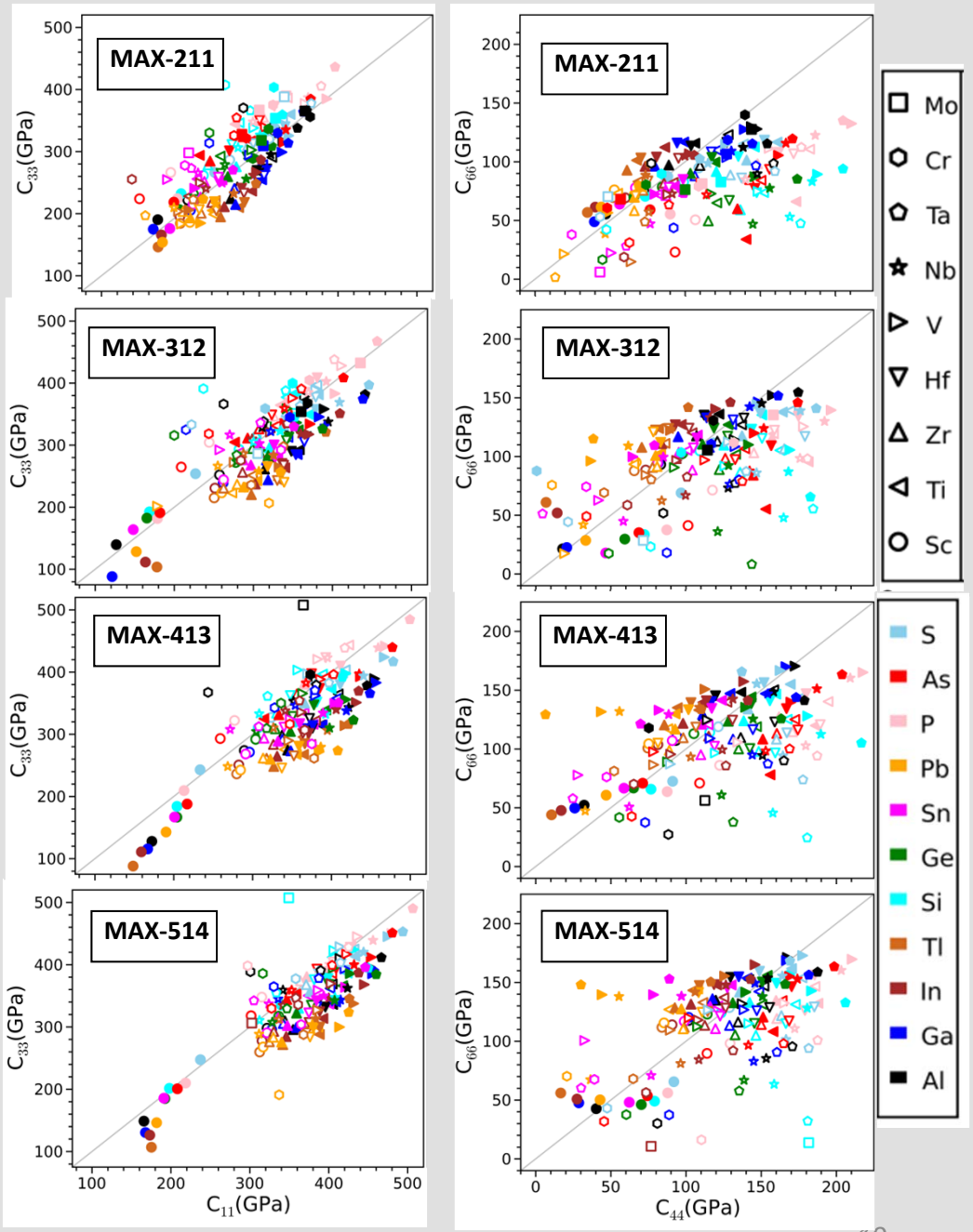
♠ Approximate linear dependence.

♠ $C_{11} \cong C33$ => isotropic.

♠ trends depending on n, more linear dependence on increasing n.

♠ Marked difference in X=C and X=N.

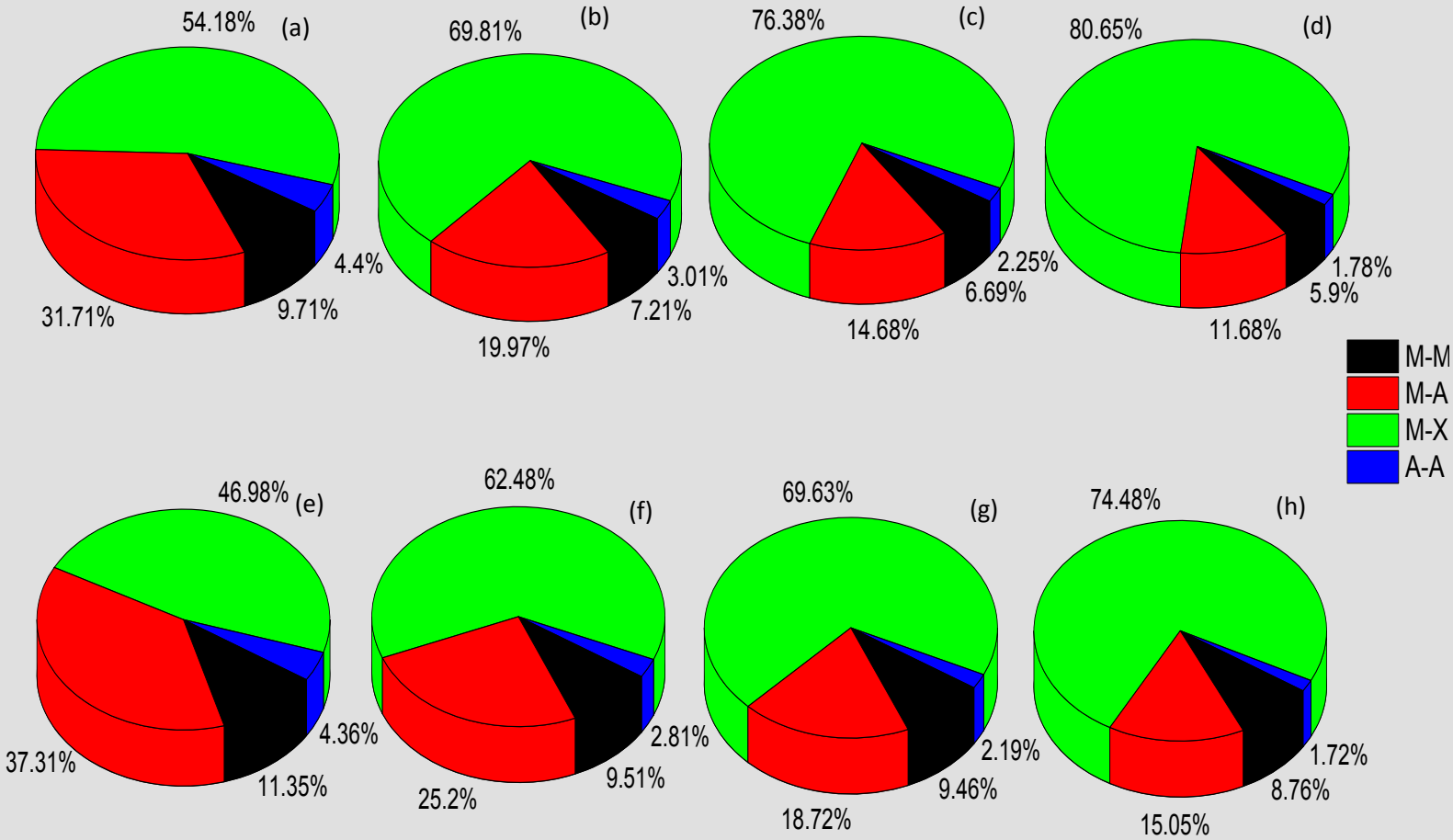
♠ Data for C_{44} vs. C_{66} more scattered and less well defined trends.



(2) Electronic Structure Results: Contributions from M-M, M-A, M-X, A-A pairs to the **total bond order** in the form of pie charts, (a) 211, (b) 312, (c) 413, (d) 514 carbides; (e) 211, F) 312, (g) 413, (h) 514 nitrides.

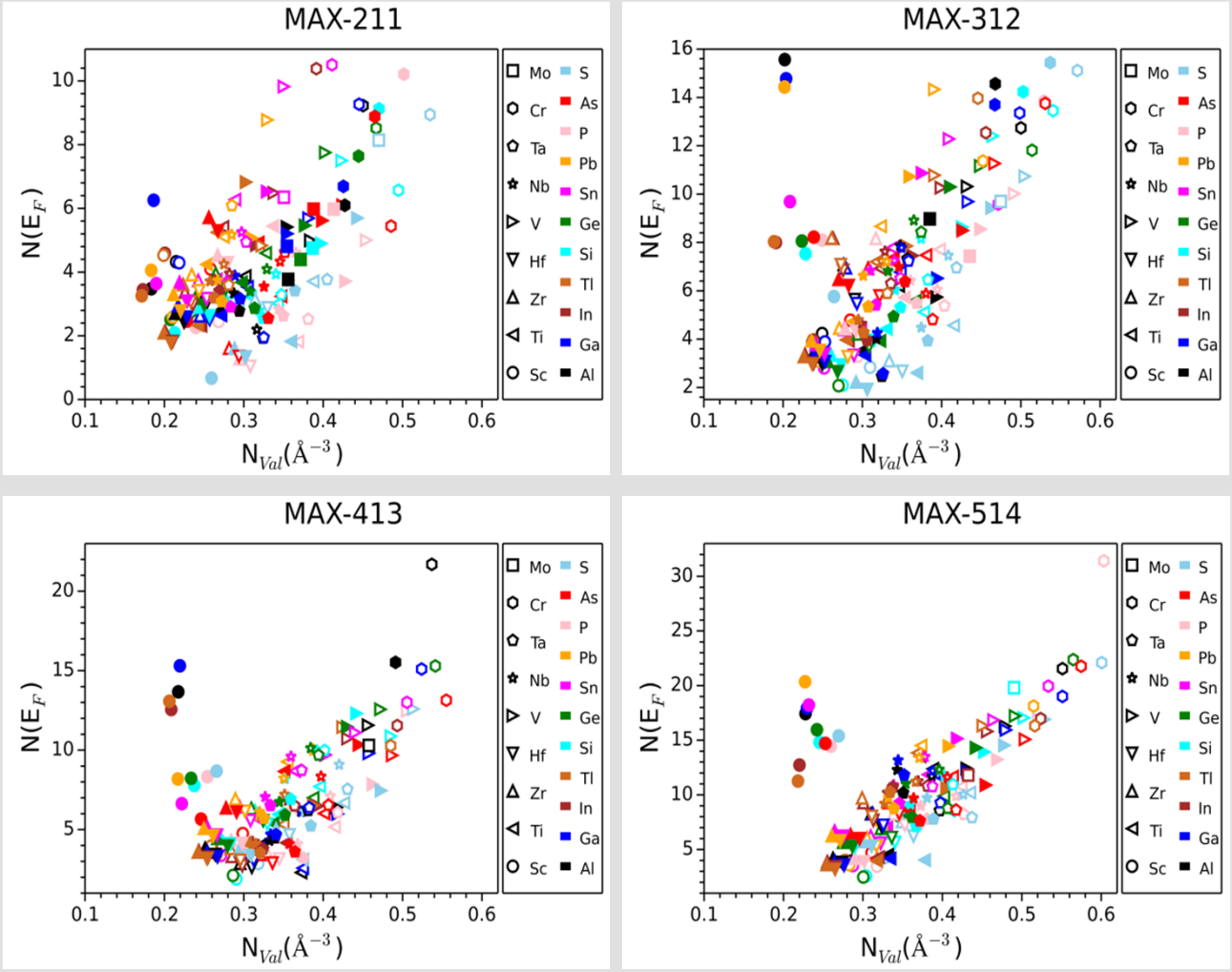
carbides

nitrides



- ♠ Relative distribution: M-X > M-A > M-M > A-A.
- ♠ Distribution different between carbides and nitrides.
- ♠ M-X more important in Carbides; M-A more important in Nitrides.

(2) Electronic Structure Results: Plot of DOS at Fermi level $N(E_F)$ against total number of valence electrons per unit volume in the crystal.



♠ $N(E_F)$ in metals and alloys, a single parameter for electronic structure.

♠ Data are scattered but have approximate linear correlation.

♠ Sc-based carbides is an exception (absences of *d* electrons).

(3) Correlation between mechanical Property and electronic structure:

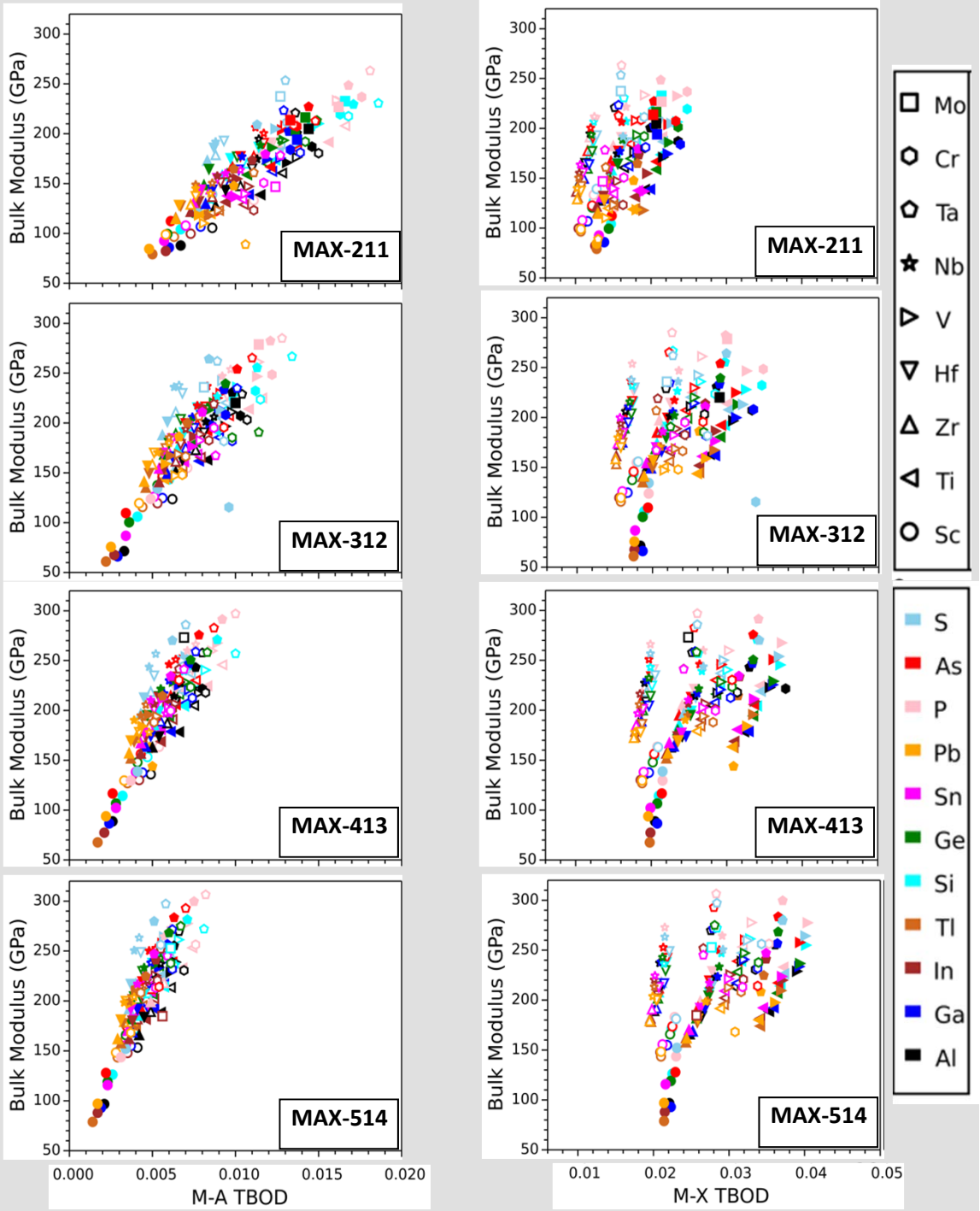
Correlation plots of bulk modulus (K) vs. M-A part of the TBOD (left) and M-X part of the TBOD (right). Other plots are not shown here.

Comments:

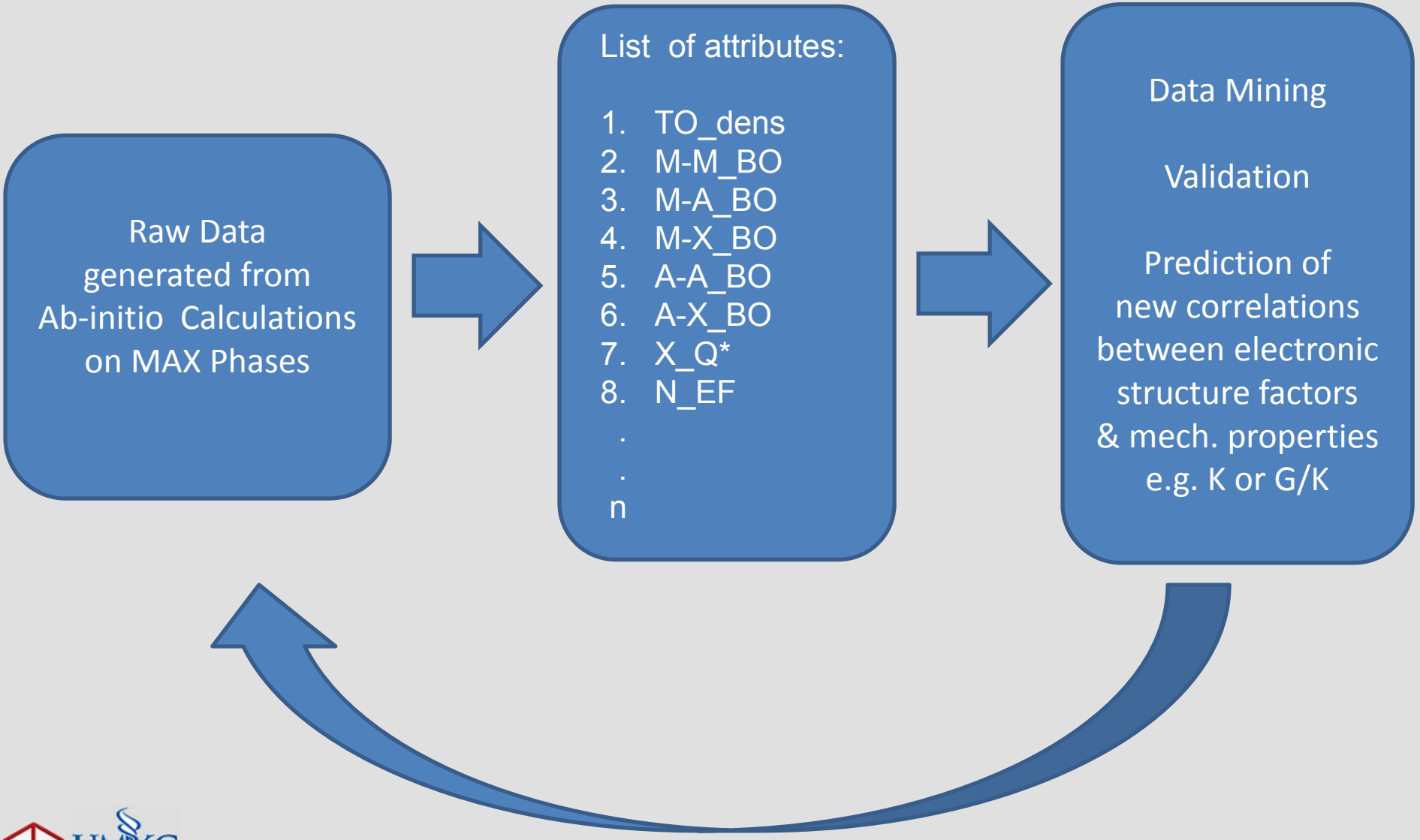
♠ K has beautiful linear correlation with M-A TBOD than M-X, but M-X has larger contribution!

♠ The slope of linear correlation increase with n.

♠ The reason is A plays a crucial role in the elastic and electronic properties of MAX phases.



Materials Informatics: ab-initio-data–Based Machine Learning & Data Mining

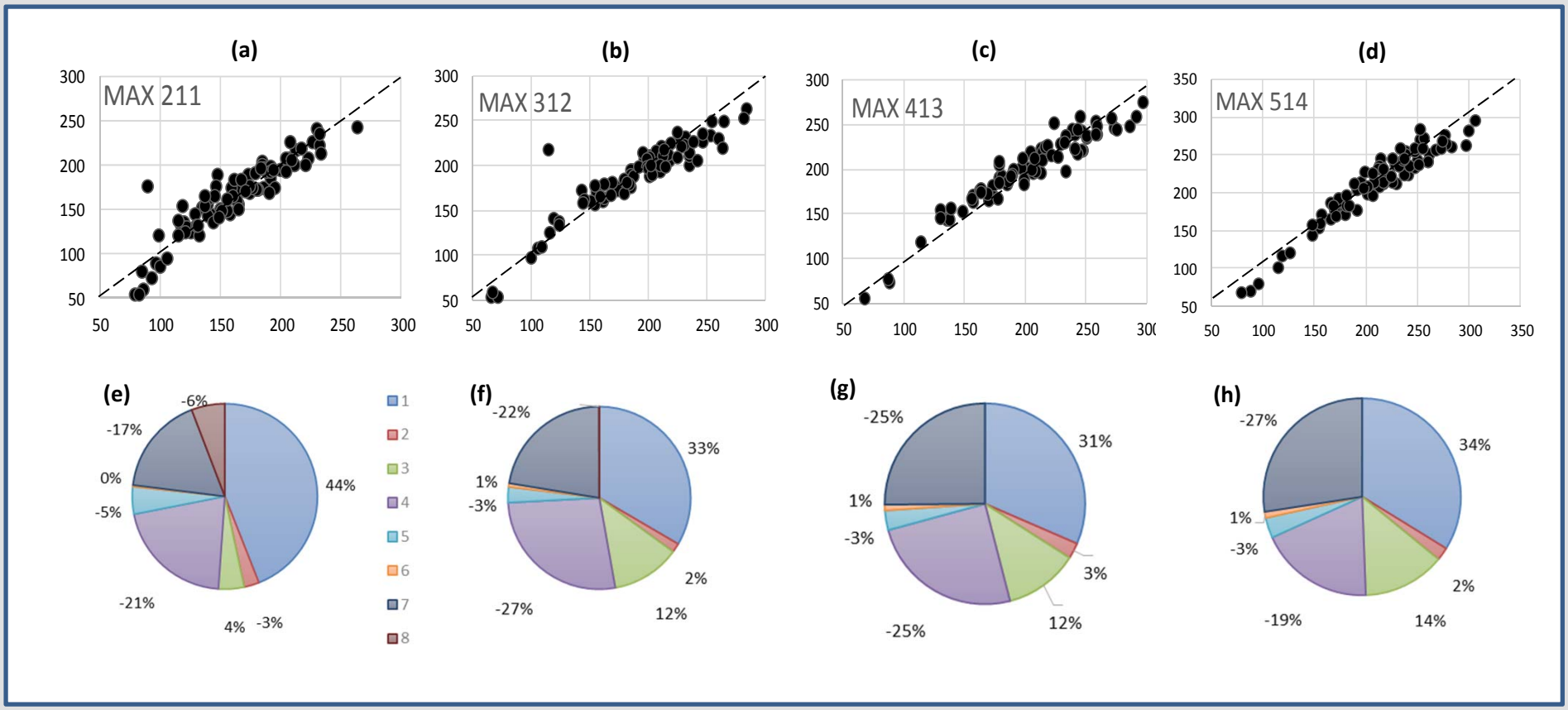


Materials Informatics: ab-initio-data–Based Machine Learning & Data Mining

♠ Based on the 665 data point we have for the MAX phases to test the efficacy of the current popular data mining algorithm:

♠ Use 50 % of the data as the training set to predict the properties of the other 50% by comparing with those calculated using *ab initio* methods.

♠ Over 90 % of predictability validates the concept of genomic approach.



a-d Comparative plots of **bulk modulus** from ab-initio DFT calculations versus that from data-mining algorithm using half of randomly chosen a) 211, b) 312, c) 413 and d) 514 MAX phases,

e-h Pie-charts showing the average relative contributions of each electronic structure factors to the predicted bulk modulus. 1 = TOBODs, 2 =M-M_BO, 3 =M-A_BO, 4 =M-X_BO, 5 =A-A_BO, 6 =A-X_BO, 7 =X_Q*, 8 =N(E_F).

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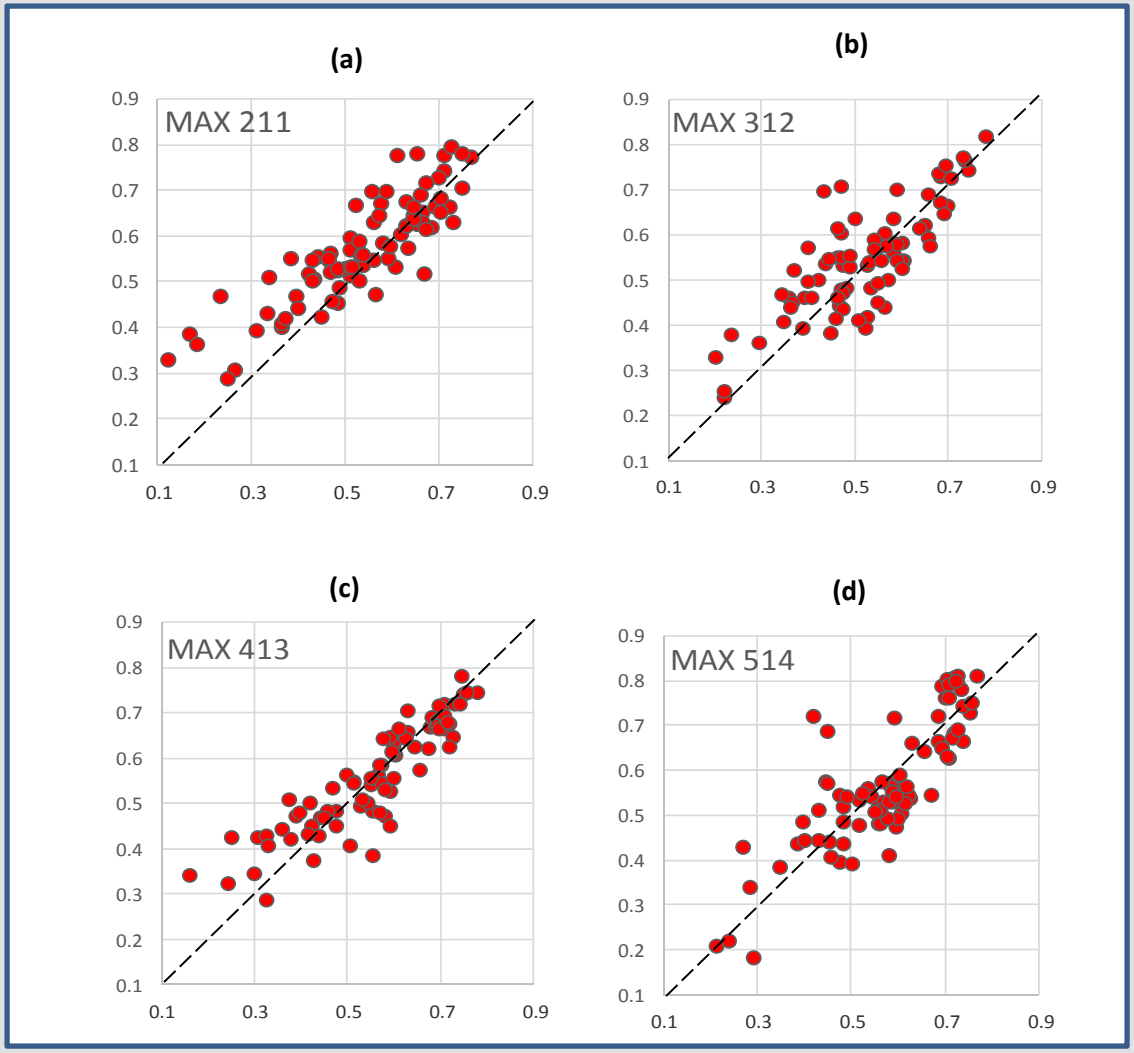


Comparative plots of **G/K** from ab-initio DFT calculations versus that from data-mining algorithm using half of randomly chosen: a) 211, b) 312, c) 413 and d) 514 MAX phases. The correlation is still impressive (> 80%)

V. Summary and Conclusions

- ♠ Large data base has been constructed for **all** MAX phases. These include both the mechanical parameters and electronic structures.
- ♠ Results consistent with experiment. The screened out phases are shown to be non-existent.
- ♠ There are noticeable trends in the nature of the mechanical properties based on their positions in the Periodic Table.
- ♠ Correlations to the electronic structure and bonding and mechanical properties has been identified. (Main goal!)
- ♠ These data base will be extremely valuable to experimentalists who try to synthesize new MAX phases in laboratories.
- ♠ This data base is used to test the algorithms for data mining and machine learning informatics in materials research.
- ♠ Quality of the database is extremely important!

We consider our NETL project to be highly successful for a purely computational project!

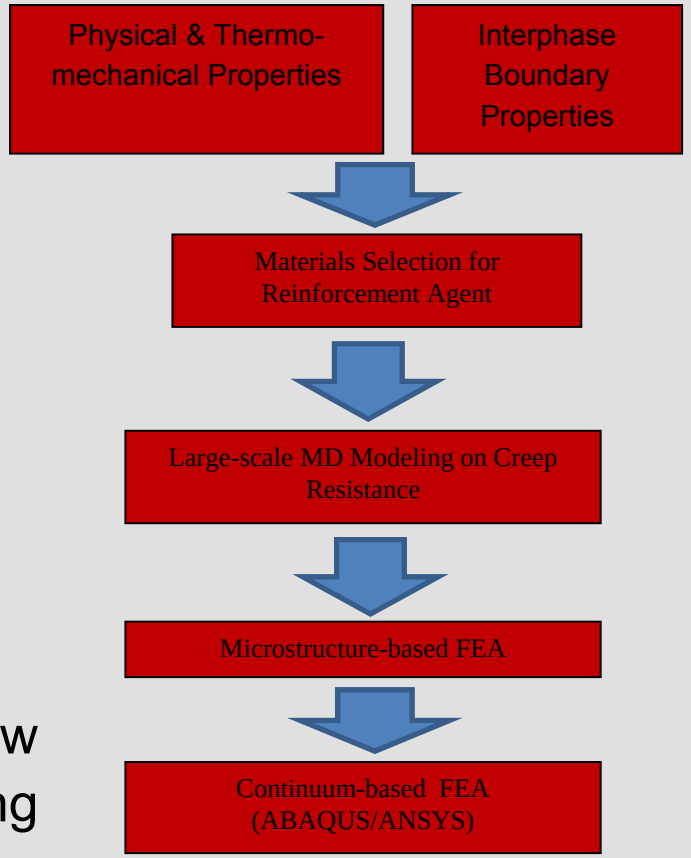
VI. Future Work

♠ Extend to solid solutions and composites in MAX phases.

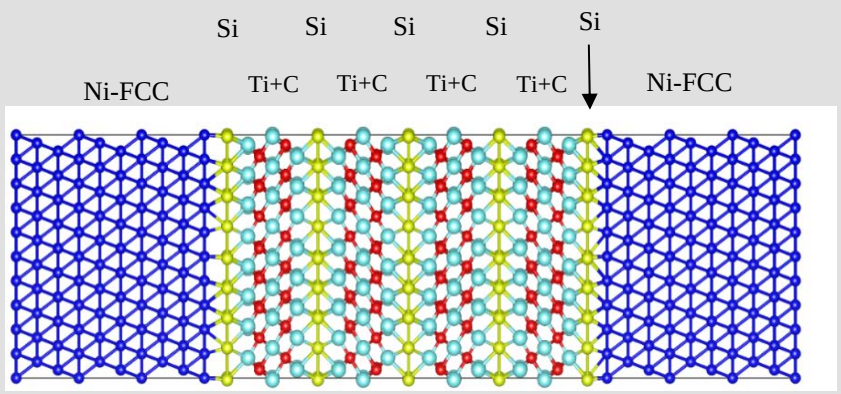
♠ Extend elements **M**, **A**, **X** and to Mxenes and MAX-like phases.

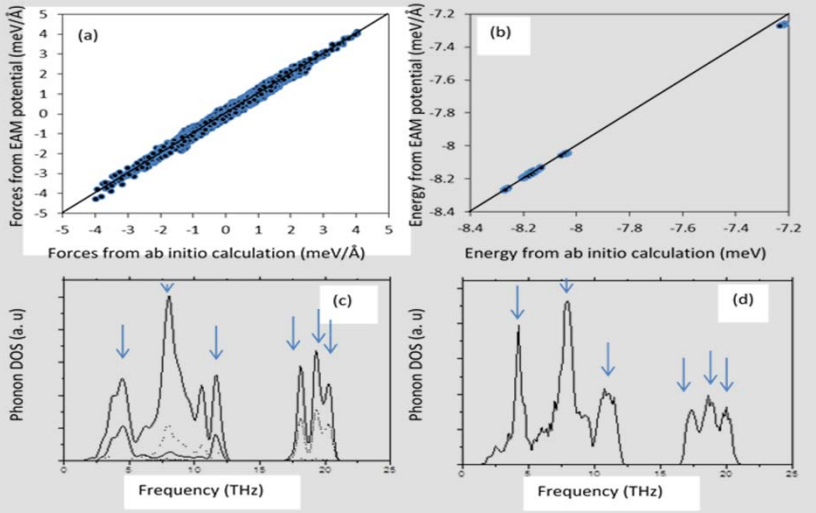
♠ Extension to include other properties such as chemical composition, corrosion resistance, thermoconductivity, optical properties, failure behavior, high temperature properties etc.

♠ We are in the process of using **genomic** approach for modeling interfaces and microstructures in Ni-based A-USC alloys to address the weldment problem in fossil energy materials by using MAX phases as strengthening agents under severe environment.

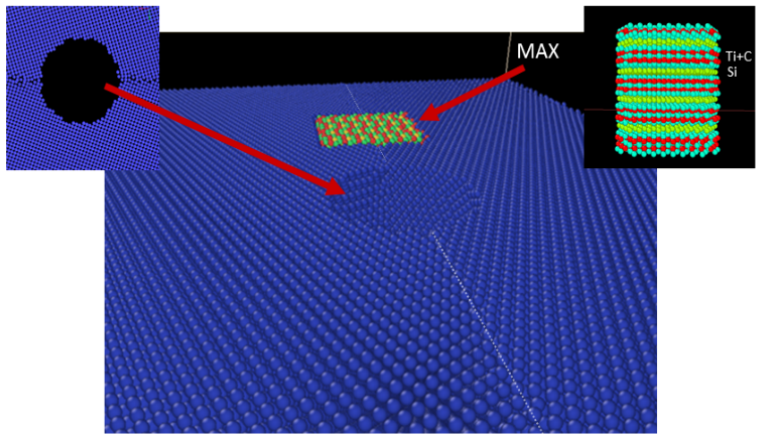


Schematics of the work flow of a new roadmap to integrate a strengthening MAX phase into A-USC alloys.

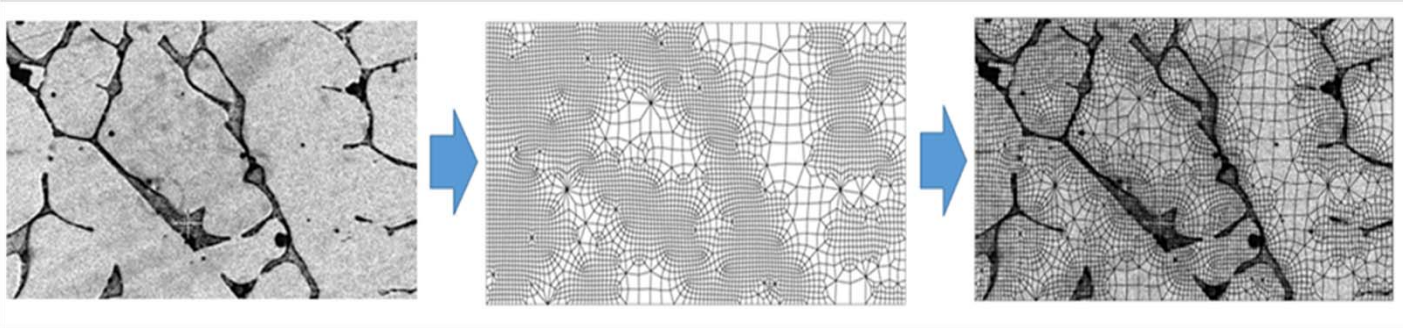




↑ Comparison **a)** Force & **b)** Total Energy. **c-d**) Phonon DOS from ab initio calculations vs. EAM potential.



← Large scale (> 1 million atom) classical MD simulation to simulate the creep resistance of MAX-reinforced HAZ.



↑ Application of atomic scale simulation to continuum model: (a) SEM micrograph of HAZ, (b) microstructure based EFM code with dense mesh, c) FEA simulation.

Thank you!

Acknowledgment:

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Ab-initio-data–Based Machine Learning and Data Mining

List of coefficients for K and G/K estimates from data-mining algorithm using a linear superposition:

$$Y = C(0) + C(1)*TB\_Dens + C(2)*M\text{-}M\_TBO + C(3)*M\text{-}A\_TBO + C(4)*M\text{-}X\_TBO + C(5)*A\text{-}A\_TBO + C(6)*A\text{-}X\_TBO + C(7)*X\_Q* + C(8)*N\_E_F$$

Y	C(0)	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)	C(8)	Correlation coefficient
K(211)	206.839	5038.871	-6.1583	3.2376	-10.1989	-28.091	100.743	-107.34	-1.2531	0.915
K(312)	187.743	3970.885	2.9706	11.89	-7.2138	-22.733	-7.2138	-82.193	-0.3916	0.9323
K(413)	230.349	4110.439	4.6844	11.738	-5.4867	-21.675	262.329	-126.40	0	0.9516
K(514)	237.707	4366.933	2.6619	12.386	-4.6634	-20.655	186.820	-116.11	-0.1278	0.9565
G/K (211)	0.2209	8.2756	-0.0261	0	-0.0384	0.0928	0.7156	0.4762	0.2209	0.8629
G/K (312)	0.1793	10.192	-0.0386	-0.0162	-0.0054	0.0606	0.6404	0.49	-0.0094	0.8189
G/K (413)	0.2108	5.505	-0.0566	0	0.0062	0.0316	0	0.43	-0.0091	0.8957
G/K (514)	-0.032	4.9746	-0.0268	0	0.0054	0.0371	0.7475	0.56	-0.0054	0.8436

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Examples of MAX phase outliers with either Sc-based or with a relatively low G/K and potentially thermodynamically stable i.e with a negative $\sum\Delta H$ or with $\sum\Delta H \leq +0.0253$ eV

MAX	G/K	CHEMICAL EQUILIBRIA	$\sum\Delta H$ (eV/atom)
Sc_3TlN_2	0.685	$Tl + Sc + 2\ ScN = Sc_3TlN_2$	- 0.0638
Ta_2GeC	0.671	$Ta_2C + TaC + TaGe_2 = 2\ Ta_2GeC$	-0.03430
Ta_3GeC_2	0.700	$Ta_2C + 3\ TaC + TaGe_2 = 2\ Ta_3GeC$	-0.04800
Ti_2AsC	0.430	$TiC + TiAs = Ti_2AsC$	+0.01854
Mo_2GeC	0.375	$3\ Mo_2C + 2\ MoGe_2 + C = 4\ Mo_2GeC$	+0.02528

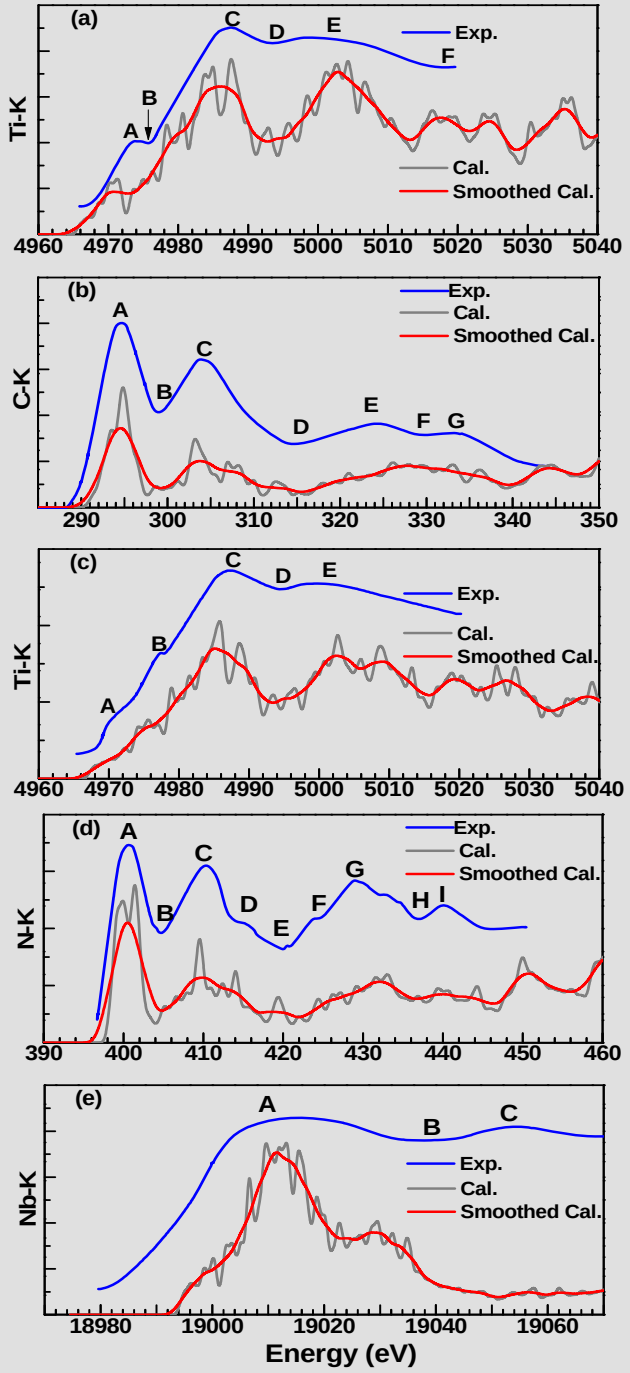
ELNES Spectral Calculation of MAX phases

♠ The spectra of Ti-K edges in Ti_2AlC and Ti_2AlN, C-K edge in Ti_2AlC, N-K edge in Ti_2AlN, and Nb-K edge in Nb_2AlC are calculated and found to be in good agreement with reported experimental measurements.

♠ More details can be found in:

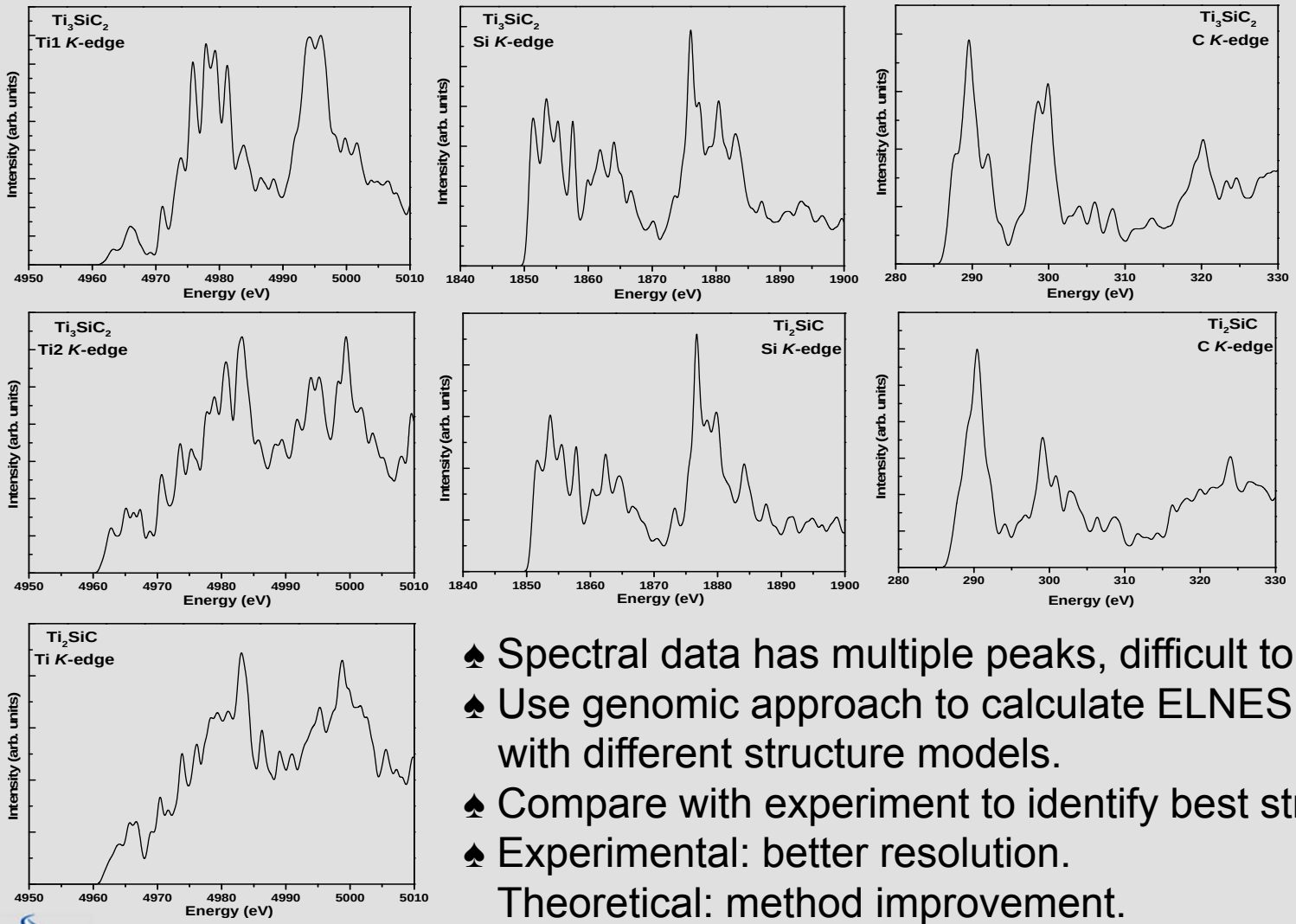
*Liaoyuan Wang, Paul Rulis, **W. Y. Ching**, "Calculation of core-level excitation in some MAX phase compounds", J. Appl. Phys. 114, 023708 (2013).*

♠ First time OLCAO-supercell method applied to metallic systems. Cole-hole effect less important than in insulators.



ELNES Spectral Calculation of MAX phases

♠ ELNES spectra for Ti_2SiC and Ti_3SiC_2 Spectra (unpublished!)



♠ Spectral data has multiple peaks, difficult to interpret.

♠ Use genomic approach to calculate ELNES spectra with different structure models.

♠ Compare with experiment to identify best structure.

♠ Experimental: better resolution.
Theoretical: method improvement.

UMKC ESG