

Atomic Environment Type (AET)

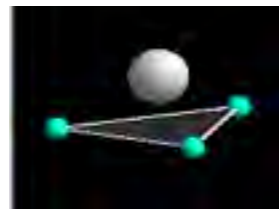
31 Most common Atomic Environment Types (AETs)



CN1



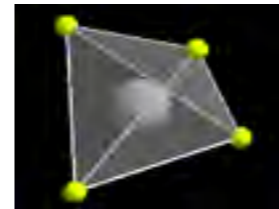
CN2



CN3



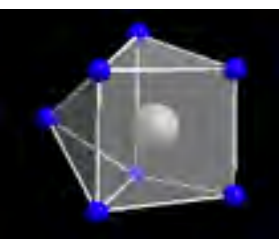
CN4



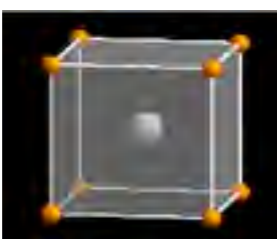
CN5



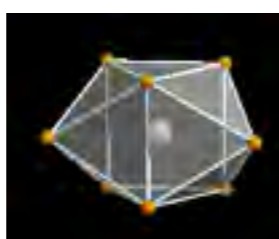
CN6



CN7



CN8



CN9



CN10



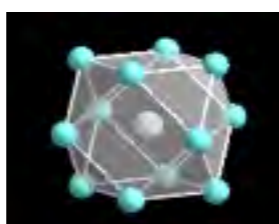
CN11



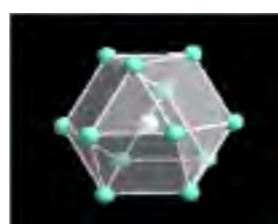
CN12



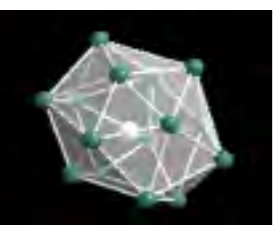
CN13



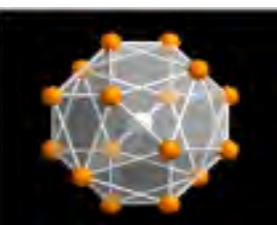
CN14



CN15



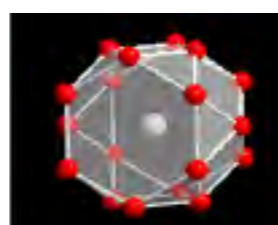
CN16



CN17



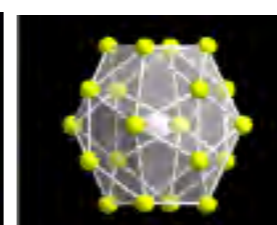
CN18



CN19

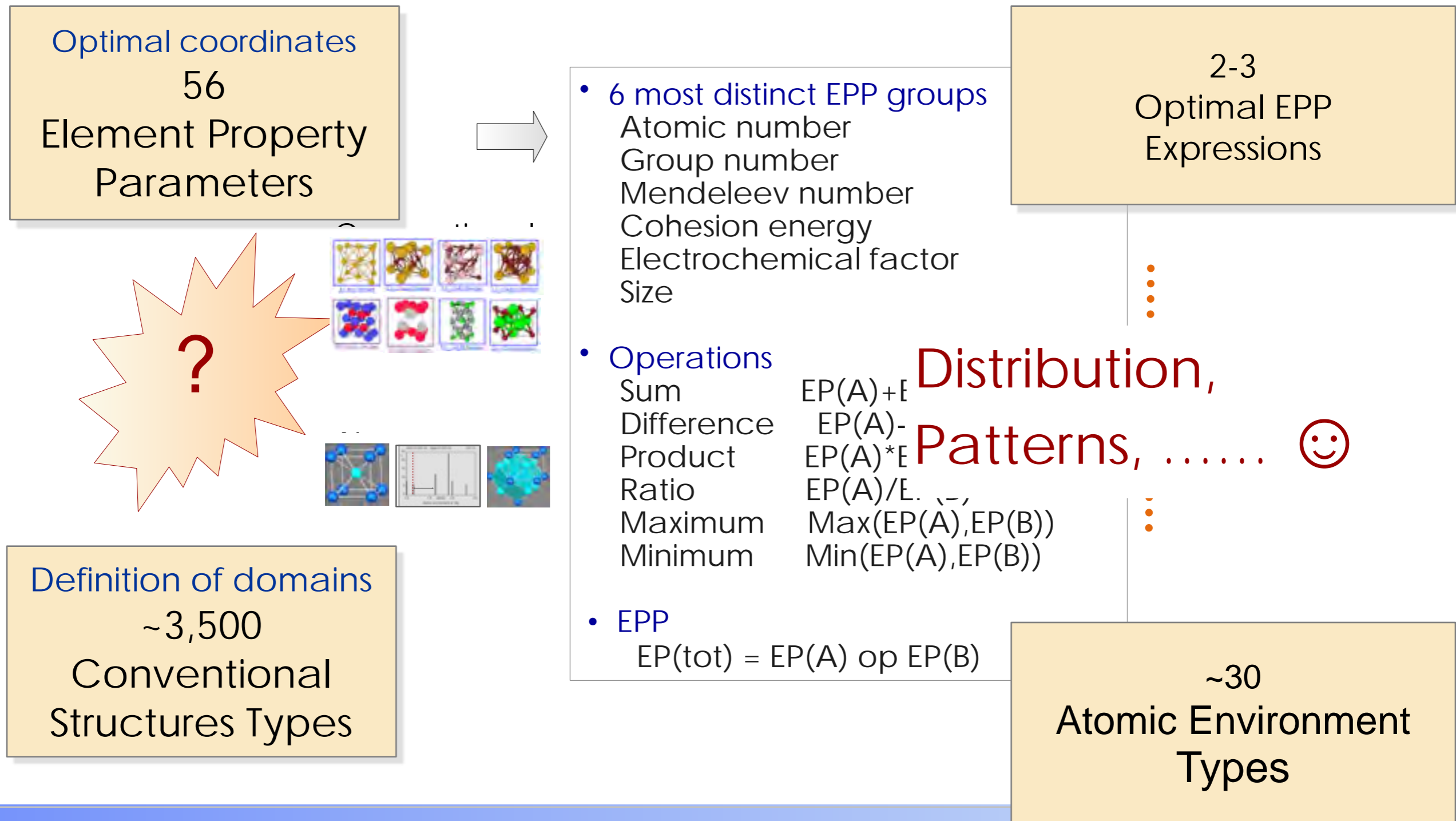


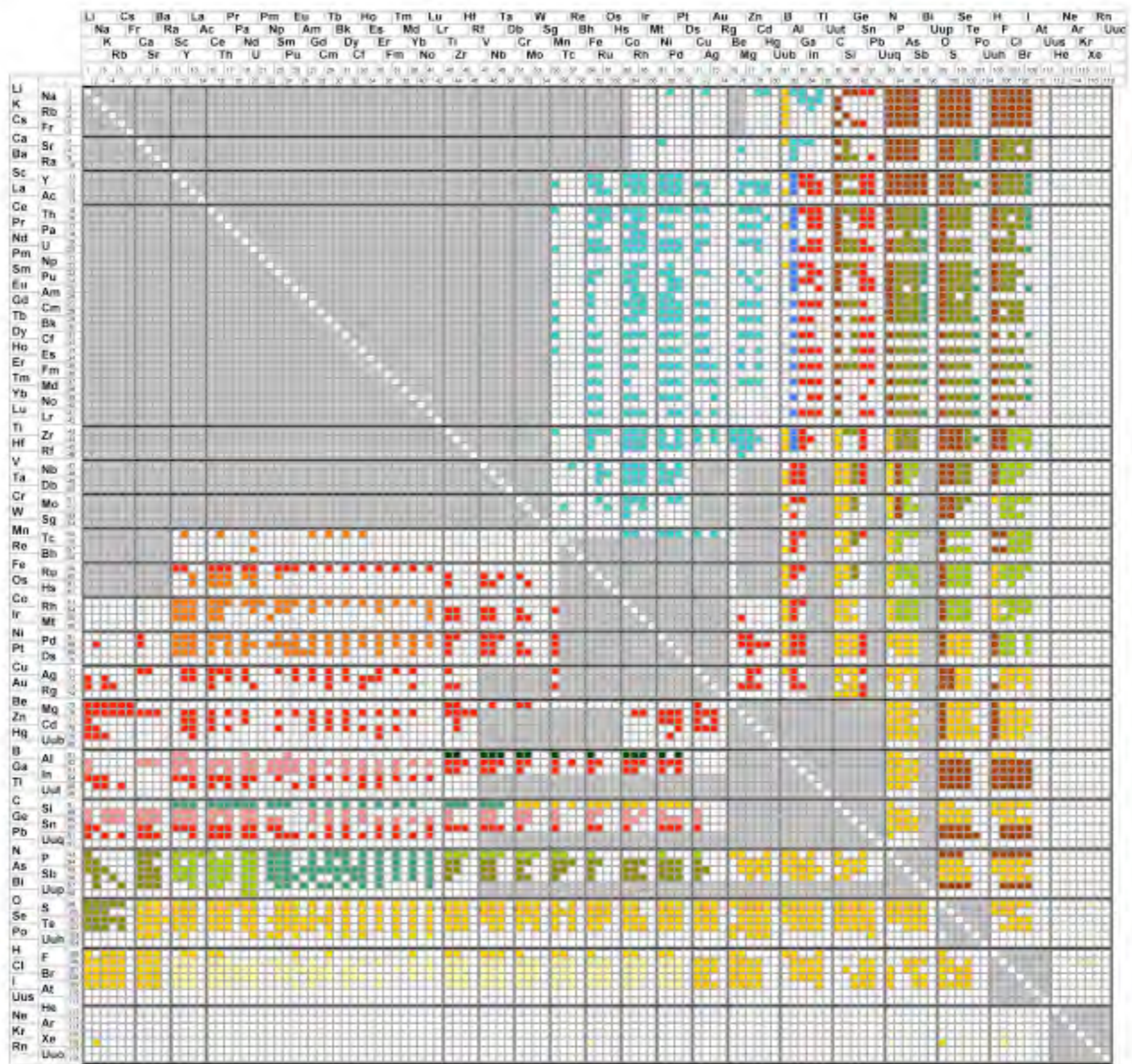
CN20



CN24

eg. Regularity between Crystal structure & Element properties





Regularities Among Binaries

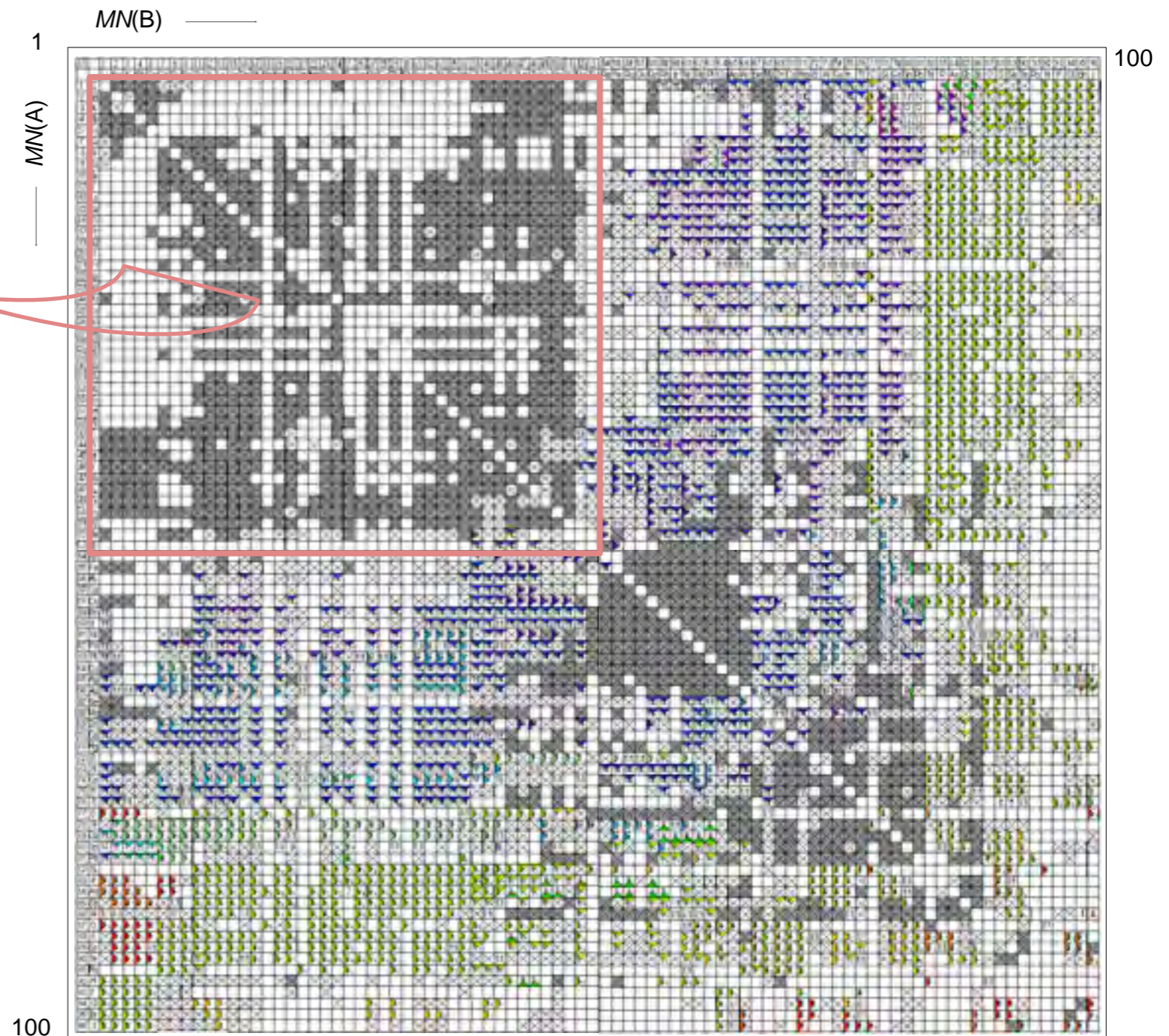
(1) Compounds Formation & (3) Structures

Mendeleev Number

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100
---	---	---	---	---	---	---	---	---	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	-----

MN(A) vs. MN(B)
Map for 1:1
Binary
Compounds (RT)

- CN 1-3
- CN 4
- CN 6 (-11)
- CN 12 (-13)
- CN 14(-18)
- ⊠ Non-former
- ⊠ Former (no 1:1)



P. Villars, Y. Chen, S. Iwata, et al. (2004)

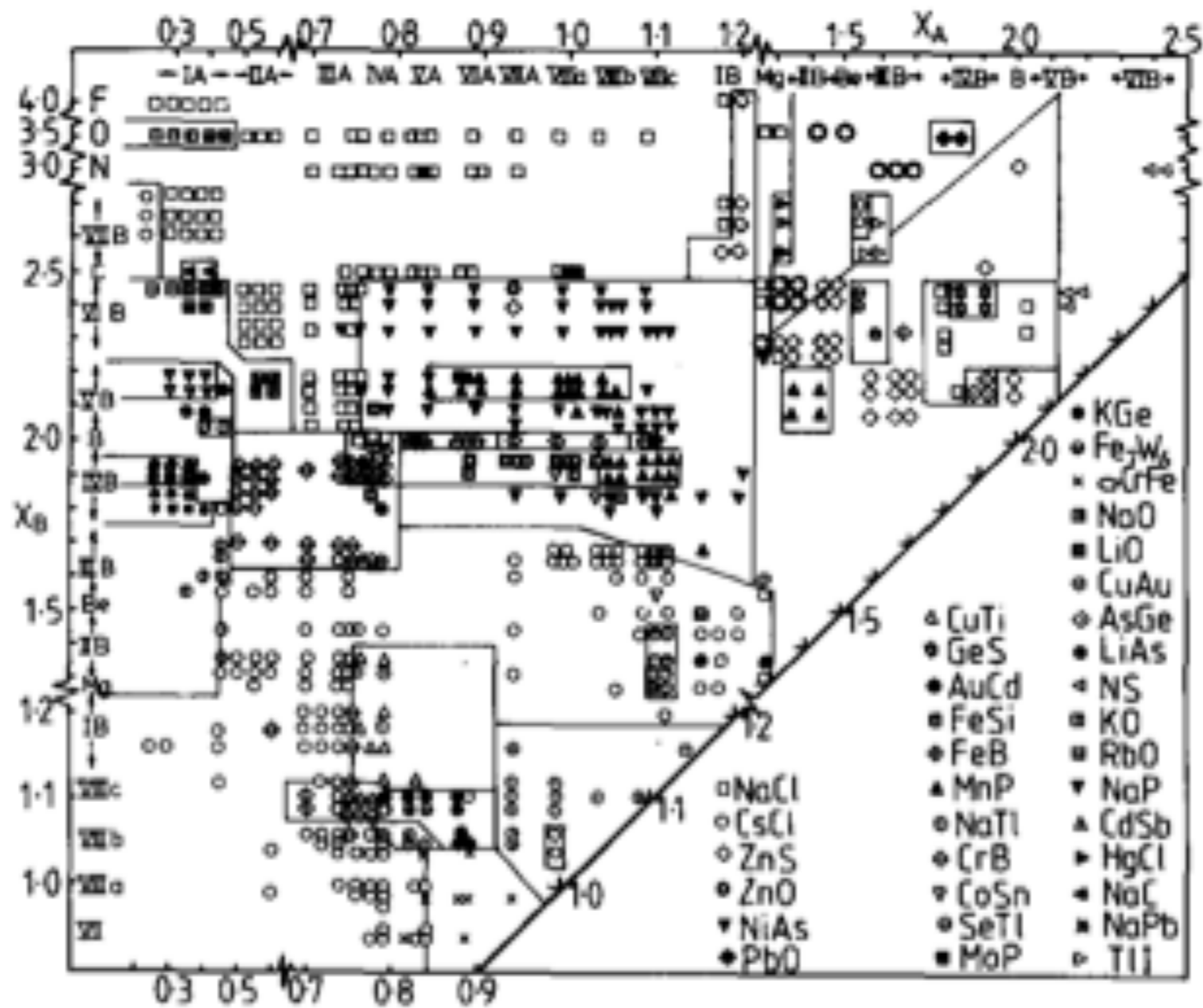
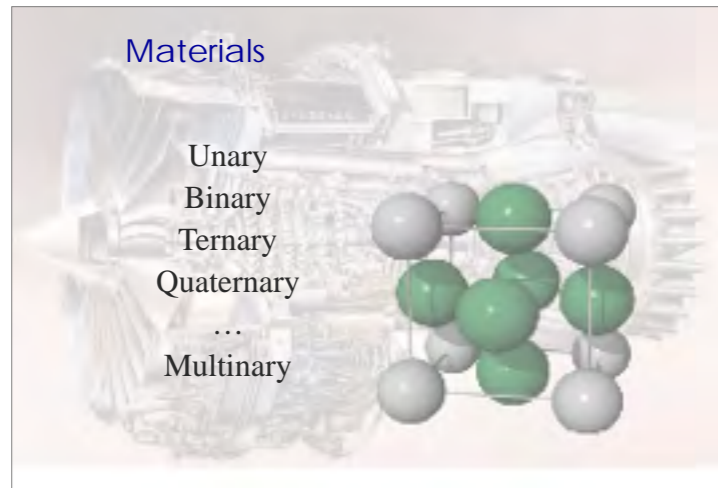
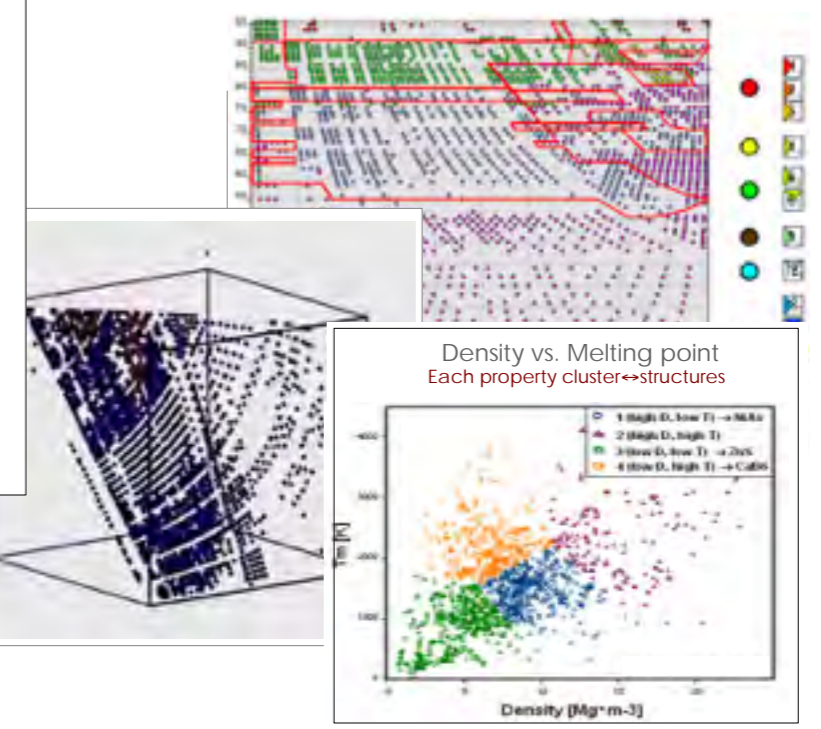
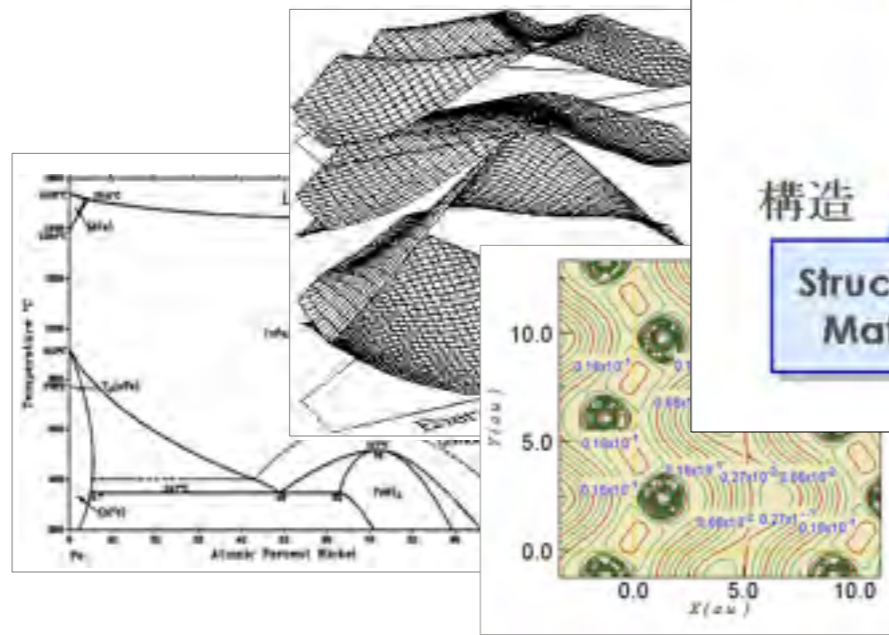
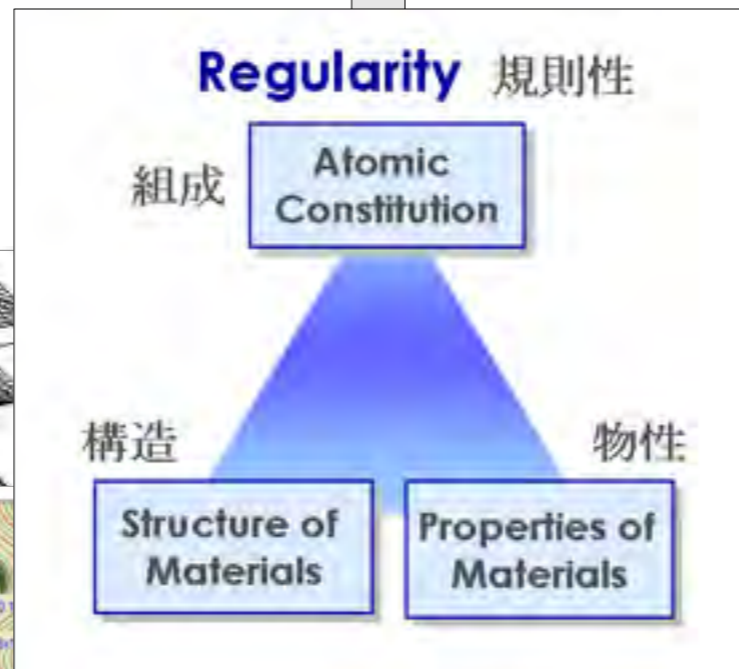
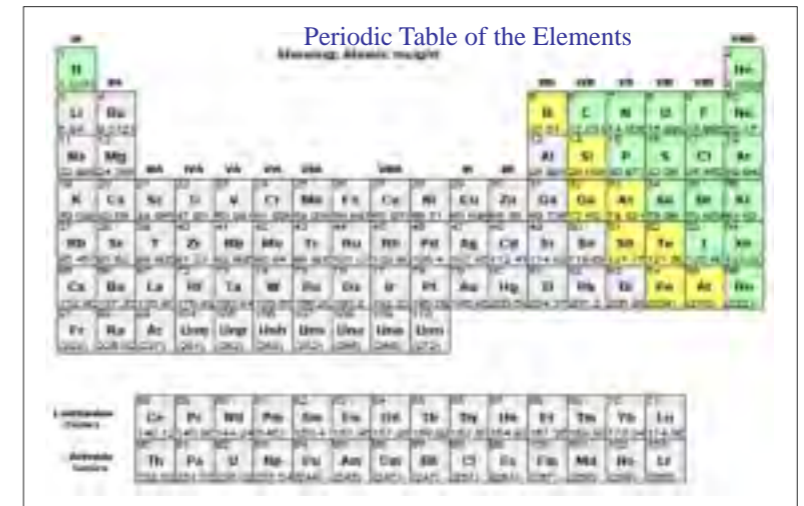
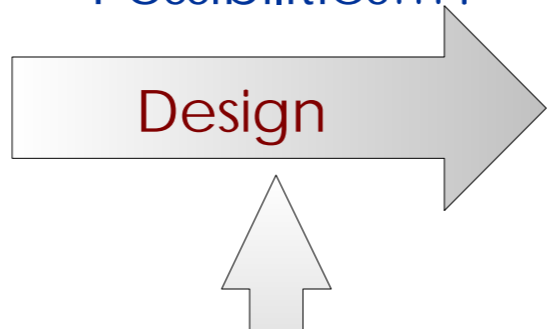


Fig. 2. The (χ_A, χ_B) structure map for 574 AB compounds.

Integrated Approach for Materials Design

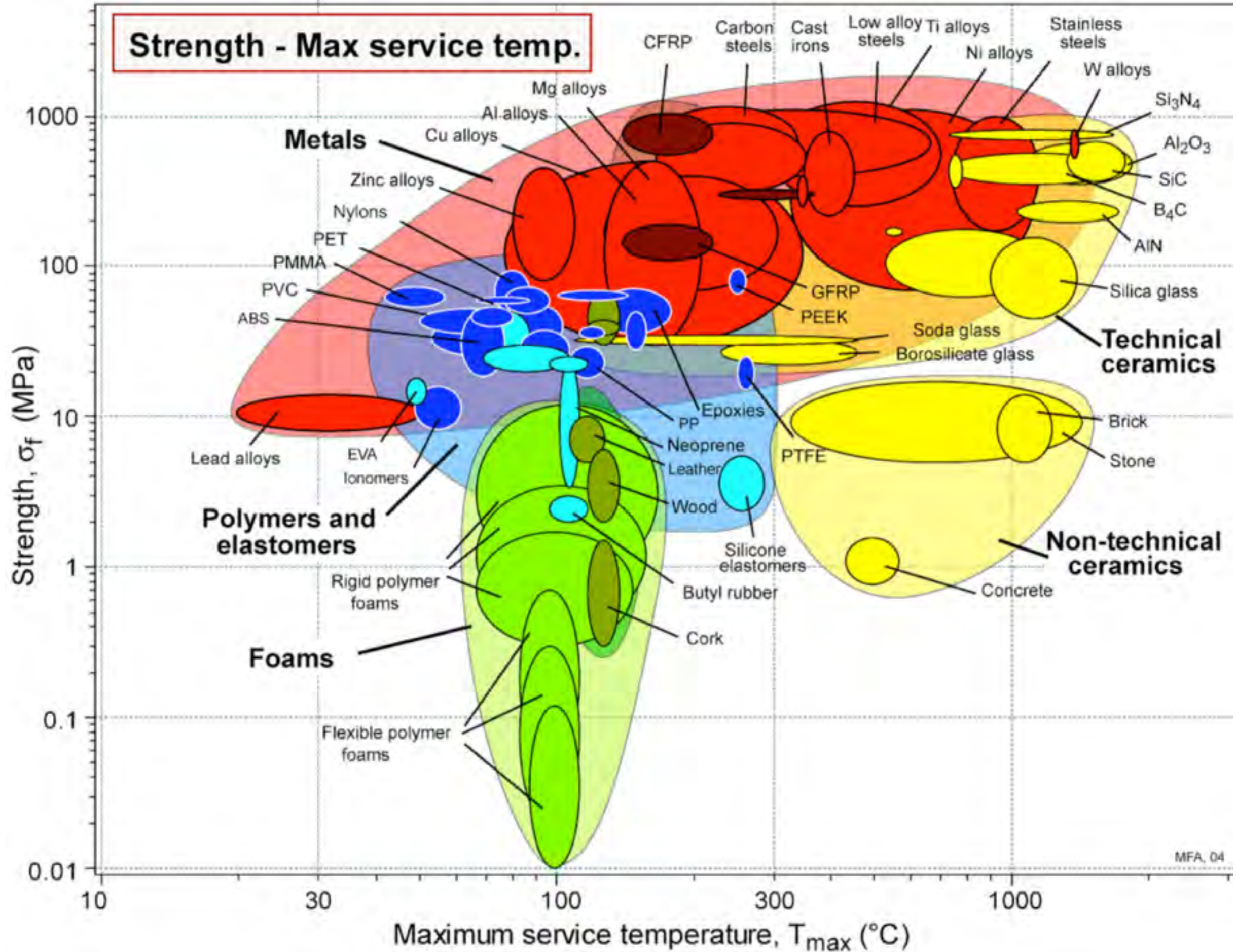


Too many Possibilities...?



Model-Driven Approach → Origin
理論計算による物質構造の本質の解明

Data-Driven Approach → Discovery
データの収集と法則の探索





アメリカ イタリア インド



ウクライナ オーストラリア オーストリア



カナダ スイス 中国



日本 ドイツ ロシア

物質・材料に関する研究状況から見た国家のパターン (五十音順)