Self-Organizing Map Technique: Data Visualization through Dimensionality Reduction

Yutaka Oya (Ph.D.)
Assistant Professor
Department of Aerospace Engineering, Tohoku University
*Currently Department of Chemistry, University of Washington

Traditional Way of Presenting Data

		Density [g/cm]	Glass transition temperature (Tg) [°C]	Yield Stress [MPa]	Young's modulus [GPa]	Tri-axial Strength [MPa]	Cure rate [%/fs]	Saturation point [%]
#1	DGEBA / DETA	1.188	145.9	216.6	2.901	174.9	57.38	84
#2	DGEBA / MPDA	1.211	210.5	253.6	3.165	177.4	49.27	75.5
#3	DGEBA / 44DDS	1.275	198.2	248.2	3.531	200.8	40.80	77.2
#4	DGEBA / 33DDS	1.273	183.4	252.9	3.303	206.3	46.05	76
#5	DGEBF / DETA	1.241	158.4	289.2	3.612	223.9	56.73	82.5
#6	DGEBF / MPDA	1.263	208.0	263.5	3.036	215.9	54.42	81.4
#7	DGEBF / 44DDS	1.298	204.1	275.6	3.068	239.5	42.14	80.7
#8	DGEBF / 33DDS	1.293	217.5	251.9	3.101	214.5	48.62	79.8
#9	TGDDM / DETA	1.205	228.3	405.7	5.095	301.5	60.49	82
#10	TGDDM / MPDA	1.217	269.4	376.9	4.925	297.0	45.55	85.4
#11	TGDDM / 44DDS	1.290	276.5	397.8	4.564	285.1	43.58	77.1
#12	TGDDM / 33DDS	1.282	307.6	388.8	5.056	265.1	49.62	78.2
#13	MTGAP / DETA	1.253	267.8	383.6	5.739	313.8	65.21	80.2
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#17	GAN/ DETA	1.216	229.2	318.7	4.395	237.8	68.48	82.5
#18	GAN / MPDA	1.245	197.9	290.7	4.159	221.3	54.83	84.8
#19	GAN / 44DDS	1.295	245.5	293.9	3.897	226.2	50.40	74.8
#20	GAN / 33DDS	1.285	243.8	283.4	3.879	219.2	38.65	80.2
#21	DGEBA / DAPNNDA	1.251	200.3	301.1	3.648	226.0	58.35	81.4
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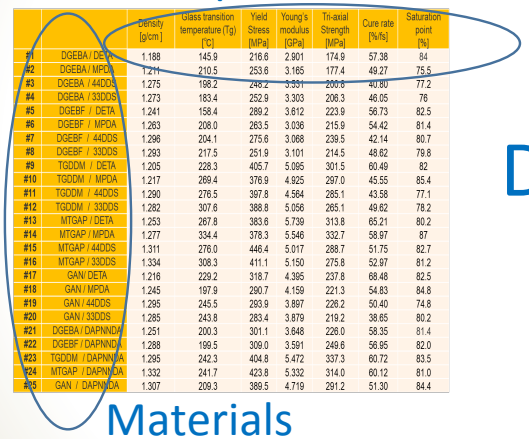
#25	GAN / DAPNNDA	1.307	209.3	389.5	4.719	291.2	51.30	84.4

Date-Base

Traditional Way of Presenting Data

Properties

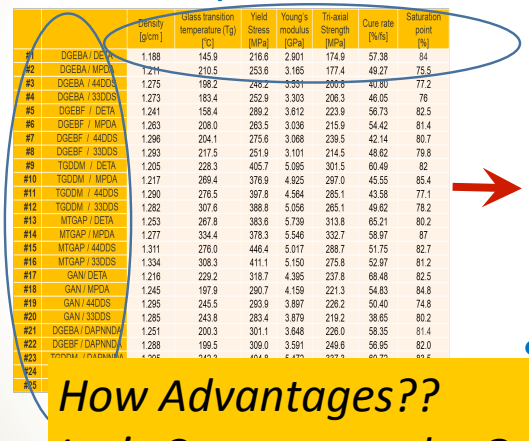


Materials

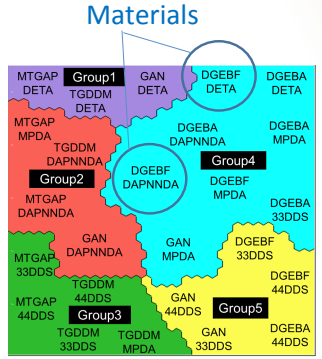
Date-Base

Self Organizing Maps

Properties



Materials



Self-Organization!

How Advantages??
Let's Compare to the Other Teqniques

Visualization Techniques

	Density [g/cm]	Glass transition temperature (Tg) [°C]	Yield Stress [MPa]	Young's modulus [GPa]	Tri-axial Strength [MPa]	Cure rate [%/fs]
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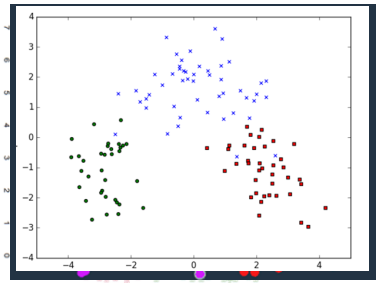
#11	1.290	276.5	397.8	4.564	285.1	43.58
#12	1.282	307.6	388.8	5.056	265.1	49.62

Data Set

Precise (quantitative) Information

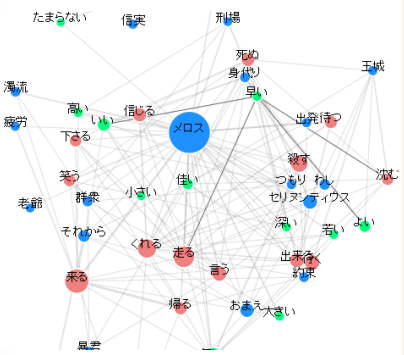
Data Set

Understanding Features



Co-Occurrence Network

Connectivity and Frequency of Each Word

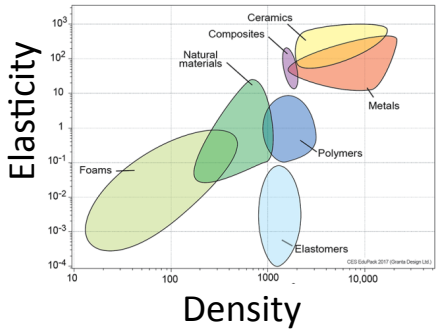


https://textmining.userlocal.jp/home/result/0c4e44ad98ed769ef4a77176009ba155

メロスは激怒した。必ず、かの邪智暴虐の王を除かなければならぬと決意した。メロスは、村の牧人である。笛を吹き、羊と遊んで暮して来た。けれども邪悪に対しては、人一倍に敏感であった。きょう未明メロスは村を出発し、野を越え山越え、十里はなれた此のシラクスの市にやって来た。メロスには父も、母も無い。女房も無い。十六の、内気な妹と二人暮しだ。この妹は、村の或る律気な一牧人を、近々、花婿として迎える事になっていた。結婚式も間近かなのである。メロスは、それゆえ、花嫁の衣裳やら祝宴の御馳走やらを買いに、はるばる市にやって来たのだ。先ず、その品々を買い集め、それから都の大路をぶらぶら歩いた。メロスには竹馬の友があった。セリヌンティウスである。今は此のシラクスの市で、石工をしている。その友を、これから訪ねて

Ashby Maps

Material Distributes on Two Dimensional Space



http://teachingresources.grantadesign.com/mikecharts/young-modulus-vs-density

Understand the relationship between Materials and Properties

Ashby Maps

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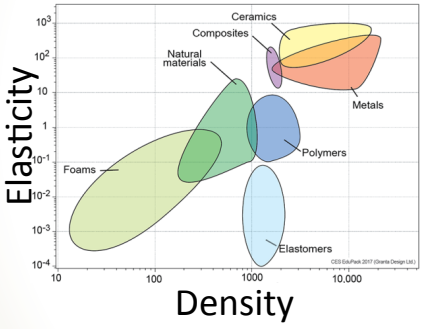

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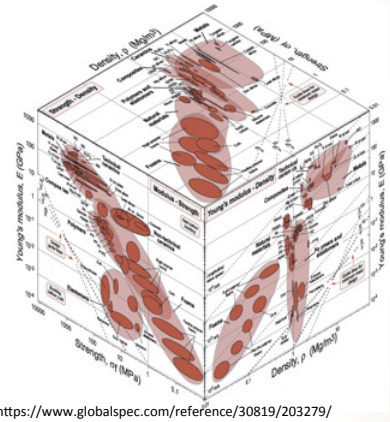
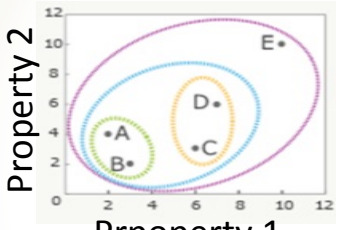
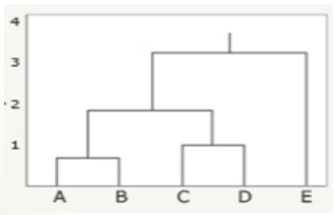


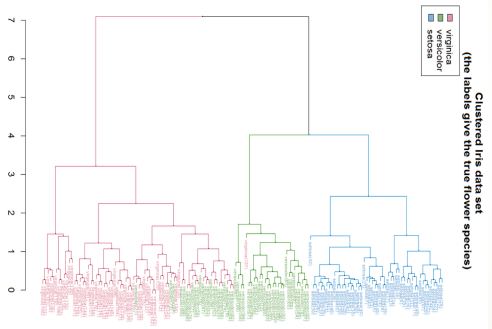
https://www.globalspec.com/reference/30819/203279/chapter-4-material-property-charts

Understand the relationship between Materials and Properties

Hierarchical Clustering
1-D Sorting depends on Similarities

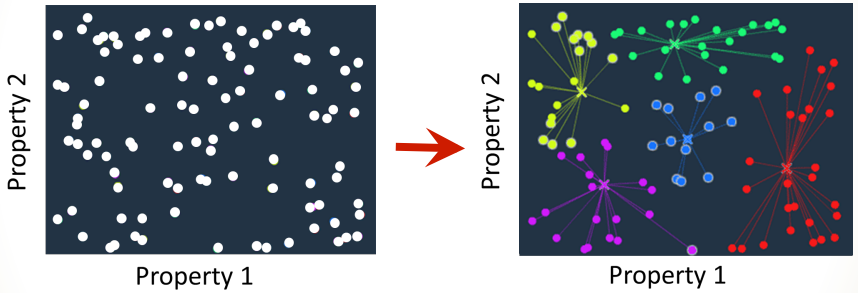






https://about.yahoo.co.jp/info/bigdata/special/2016/05/app/

K-Means Method
Clustering method for Dispersed data



http://tech.nitoyon.com/ja/blog/2009/04/09/kmeans-visualise/

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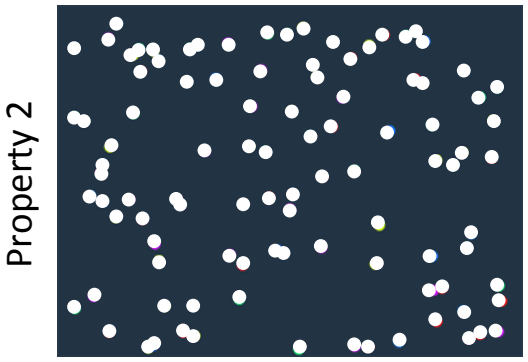

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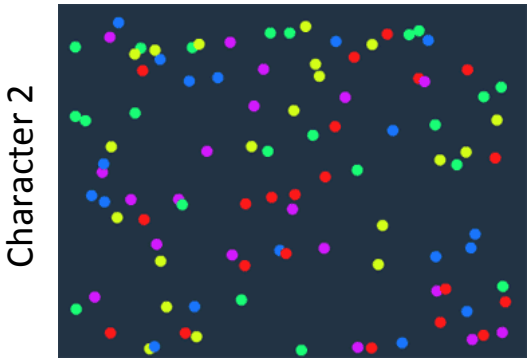

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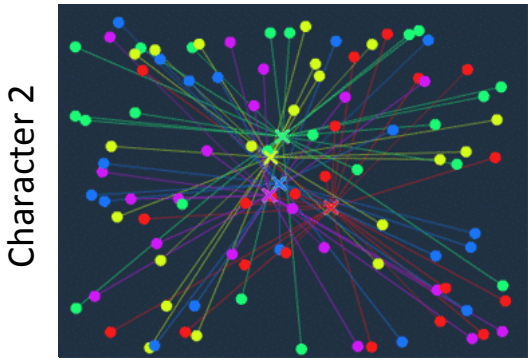

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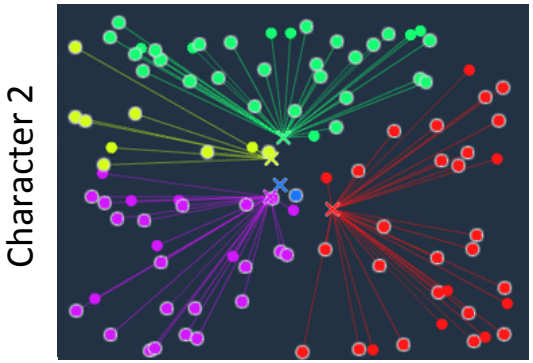

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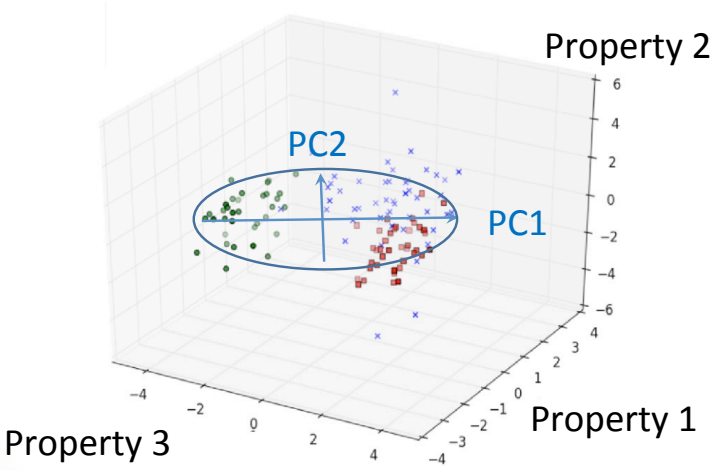
Principal component analysis

Dimensionally Reduction



http://costudyinfodatabase.nagoya/2017/07/01/

Principal component analysis

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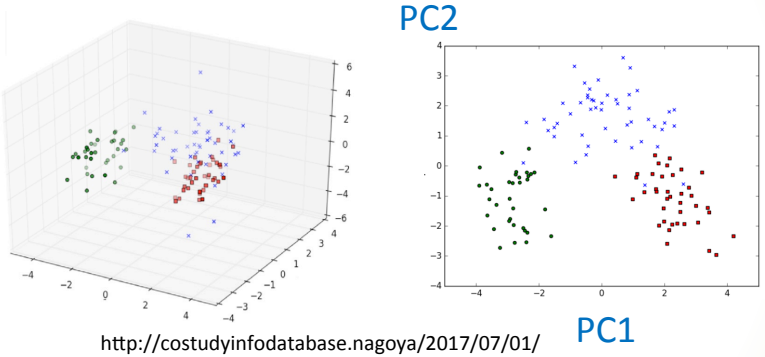

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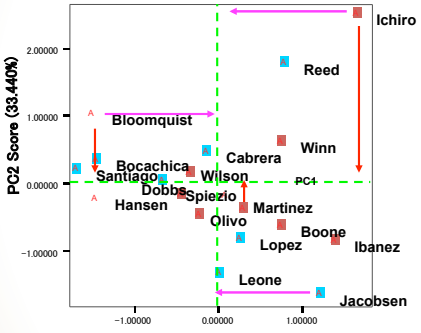
3Dimension → 2Dmension

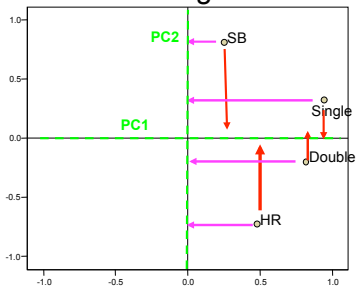
Principal component analysis

Dimensionally Reduction

Score plot



Loading Plot



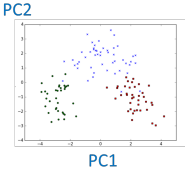
Ichiro : Good baseball player with speed

Jacobsen : Powerful but slow

Martinez : Good timing to retire

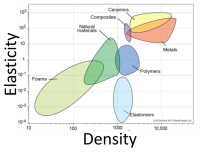
Summery of Visualization Techniques

- Dimensionally Reduction



- Clustering

- 1 to 1 Relation between Materials and Properties



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Summery of Visualization Techniques

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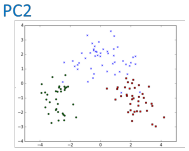

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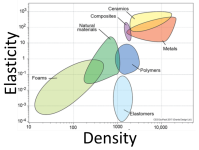

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Self-Organizing Maps

Overview of Self Organizing Maps (SOM)

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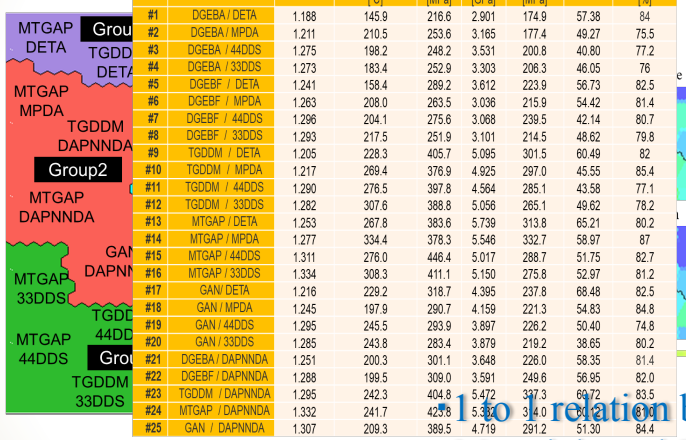
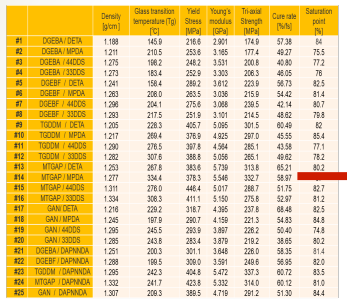
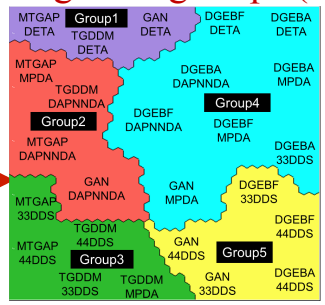
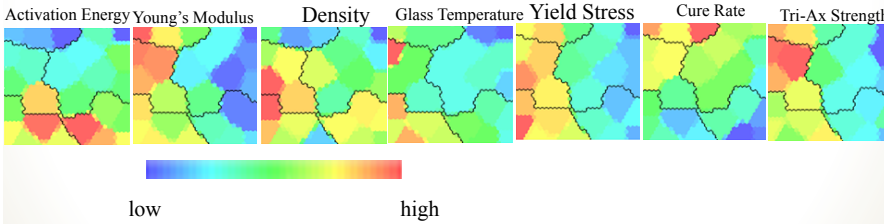


1 to 1 relation between Materials and Properties

Over View of Self Organizing Maps (SOM)







Overview of SOM

7 Properties (7dimension)

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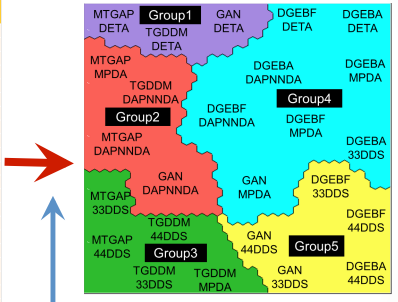
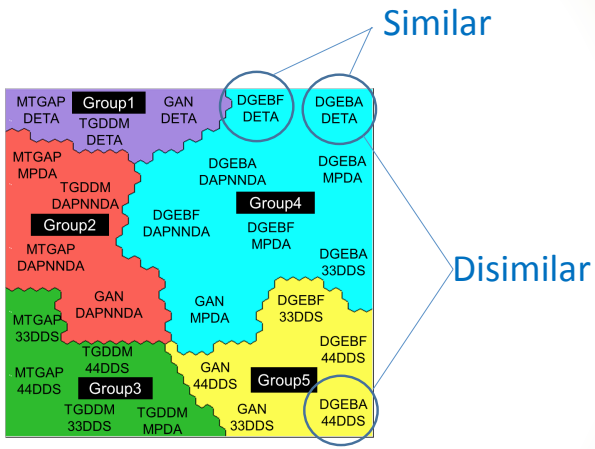
#16	MTGAP / 33DDS	1.334	308.3	411.1	5.150	275.8	52.97	81.2
#17	GAN/ DETA	1.216	229.2	318.7	4.395	237.8	68.48	82.5
#18	GAN / MPDA	1.245	197.9	290.7	4.159	221.3	54.83	84.8
#19	GAN / 44DDS	1.295	245.5	293.9	3.897	226.2	50.40	74.8
#20	GAN / 33DDS	1.285	243.8	283.4	3.879	219.2	38.65	80.2
#21	DGEBA / DAPNNDA	1.251	200.3	301.1	3.648	226.0	58.35	81.4
#22	DGEBF / DAPNNDA	1.288	199.5	309.0	3.591	249.6	56.95	82.0
#23	TGDDM / DAPNNDA	1.295	242.3	404.8	5.472	337.3	60.72	83.5
#24	MTGAP / DAPNNDA	1.332	241.7	423.8	5.332	314.0	60.12	81.0
#25	GAN / DAPNNDA	1.307	209.3	389.5	4.719	291.2	51.30	84.4



- Dimensionally Reduction: 7D→2D

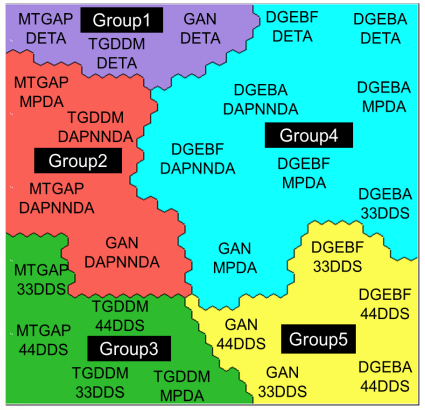
Overview of SOM

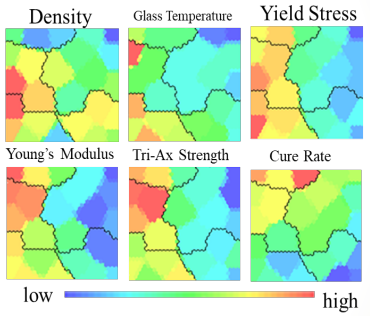
Color Clustering



- Clustering and Sorting depending on Similarity

Overview of SOM



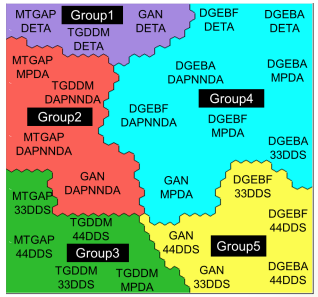


- 1 to 1 relation between Materials and Properties

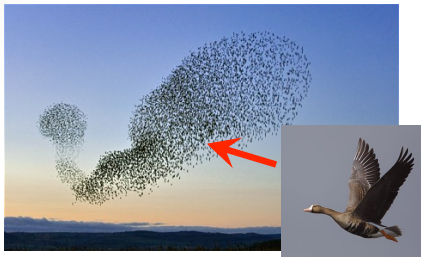
Algorithm of Self-Organization

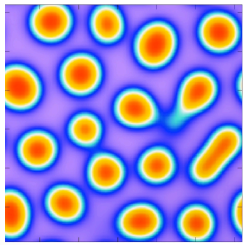
How to Organize?

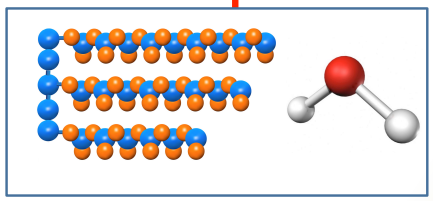
		Density [g/cm³]	Glass transition temperature (Tg) [°C]	Yield Stress [MPa]	Young's modulus [GPa]	Tri-axial Strength [MPa]	Cure rate [%/fs]	Saturation point [%]
#1	DGEBA / DETA	1.188	145.9	216.6	2.901	174.9	57.38	84
#2	DGEBA / MPDA	1.211	210.5	253.6	3.165	177.4	49.27	75.5
#3	DGEBA / 44DDS	1.275	198.2	248.2	3.531	200.8	40.80	77.2
#4	DGEBA / 33DDS	1.273	183.4	252.9	3.303	206.3	46.05	76
#5	DGEBF / DETA	1.241	158.4	289.2	3.612	223.9	56.73	82.5
#6	DGEBF / MPDA	1.263	208.0	263.5	3.036	215.9	54.42	81.4
#7	DGEBF / 44DDS	1.296	204.1	275.6	3.068	239.5	42.14	80.7
#8	DGEBF / 33DDS	1.293	217.5	251.9	3.101	214.5	48.62	79.8
#9	TGDDM / DETA	1.205	228.3	405.7	5.095	301.5	60.49	82
#10	TGDDM / MPDA	1.217	269.4	376.9	4.925	297.0	45.55	85.4
#11	TGDDM / 44DDS	1.290	276.5	397.8	4.564	285.1	43.58	77.1
#12	TGDDM / 33DDS	1.282	307.6	388.8	5.056	265.1	49.62	78.2
#13	MTGAP / DETA	1.253	287.9	383.6	5.739	313.8	65.21	80.2
#14	MTGAP / MPDA	1.277	334.4	378.3	5.546	332.7	58.97	87
#15	MTGAP / 44DDS	1.311	276.0	446.4	5.017	288.7	51.75	82.7
#16	MTGAP / 33DDS	1.334	308.3	411.1	5.150	275.8	52.97	81.2
#17	GAN/ DETA	1.216	229.2	318.7	4.395	237.8	68.48	82.5
#18	GAN / MPDA	1.245	197.9	290.7	4.159	221.3	54.83	84.8
#19	GAN / 44DDS	1.295	245.5	293.9	3.897	226.2	50.40	74.8
#20	GAN / 33DDS	1.285	243.8	283.4	3.879	219.2	38.65	80.2
#21	DGEBA / DAPNNDA	1.251	200.3	301.1	3.648	228.0	58.35	81.4
#22	DGEBF / DAPNNDA	1.288	199.5	309.0	3.591	249.6	56.95	82.0
#23	TGDDM / DAPNNDA	1.295	242.3	404.8	5.472	337.3	60.72	83.5
#24	MTGAP / DAPNNDA	1.332	241.7	423.8	5.332	314.0	60.12	81.0
#25	GAN / DAPNNDA	1.307	209.3	389.5	4.719	291.2	51.30	84.4



Self Organization







Algorithm of SOM : Data Vectorization

	Density [g/cm]	Glass transition temperature (Tg) [℃]	Yield Stress [MPa]	Young's modulus [GPa]	Tri-axial Strength [MPa]	Cure rate [%/fs]
#1	1.188	145.9	216.6	2.901	174.9	57.38
#2	1.211	210.5	253.6	3.165	177.4	49.27
#3	1.275	198.2	248.2	3.531	200.8	40.80
#4	1.273	183.4	252.9	3.303	206.3	46.05
#5	1.241	158.4	289.2	3.612	223.9	56.73
#6	1.263	208.0	263.5	3.036	215.9	54.42
#7	1.296	204.1	275.6	3.068	239.5	42.14
#8	1.293	217.5	251.9	3.101	214.5	48.62
#9	1.205	228.3	405.7	5.095	301.5	60.49
#10	1.217	269.4	376.9	4.925	297.0	45.55
#11	1.290	276.5	397.8	4.564	285.1	43.58
#12	1.282	307.6	388.8	5.056	265.1	49.62

$x_i = (a_i\ b_i\ c_i\ d_i\ e_i\ f_i)$

density

Glass transition temperature

Yield Stress

Young's modulus

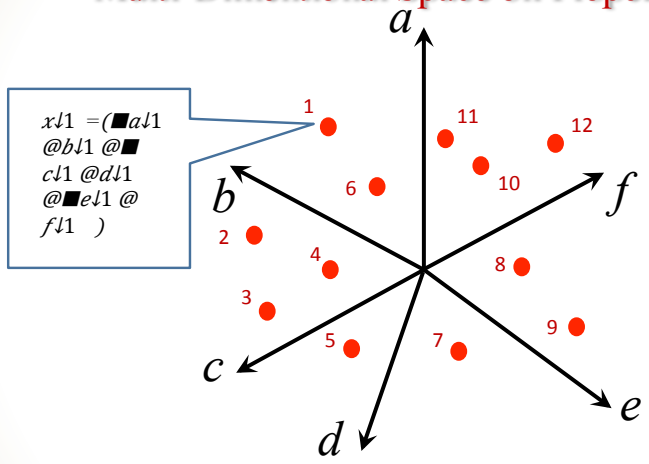
Tri-axial Strength

Cure rate

i (1 ~ 12) :Materials $a \sim f$:Properties

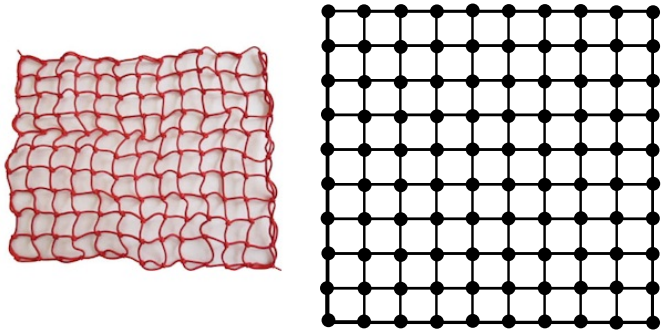
Algorithm of SOM : Multi-Dimentional Space on Properties

$x_1 = (a_1\ b_1\ c_1\ d_1\ e_1\ f_1)$

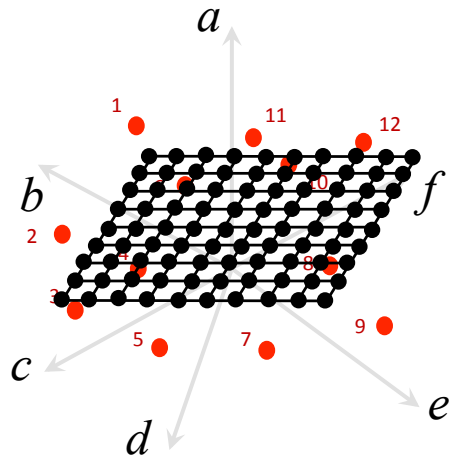


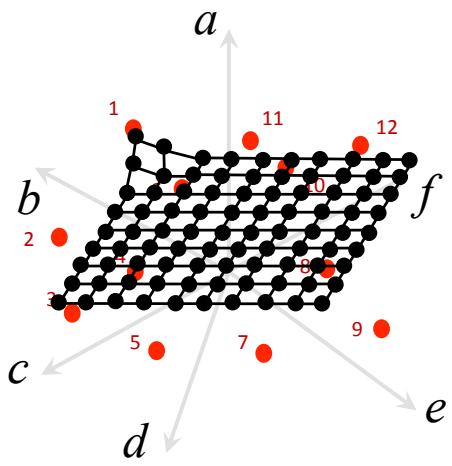
$a \sim f$:Properties

Two Dimensional Mesh Structure



Each connection can deform

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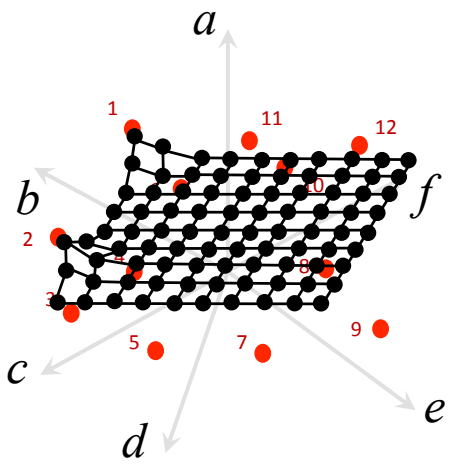
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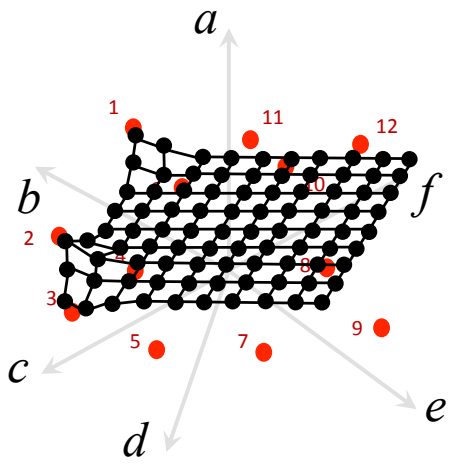
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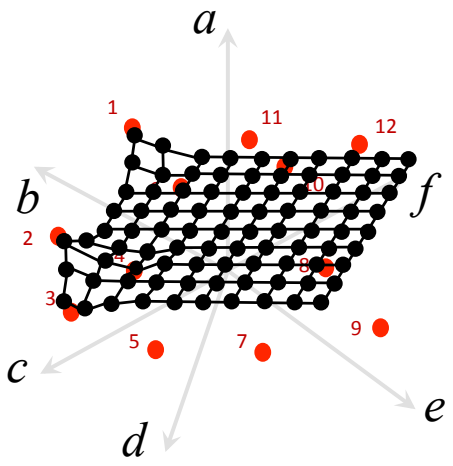
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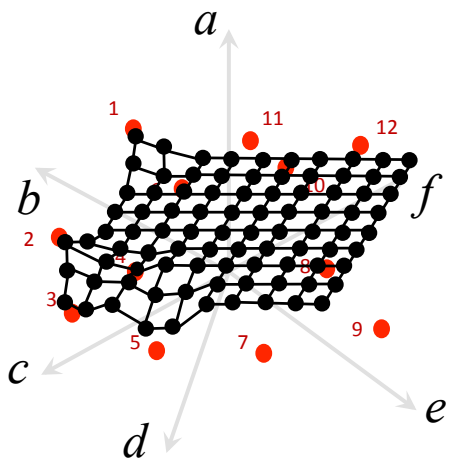
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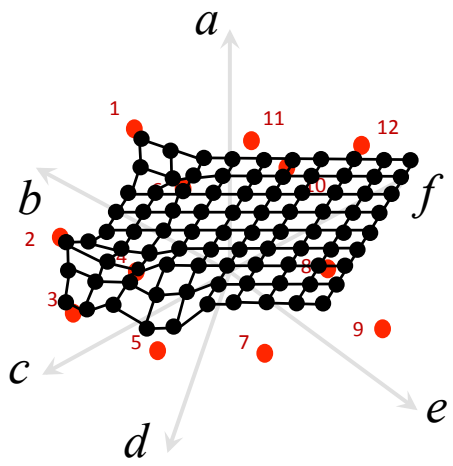
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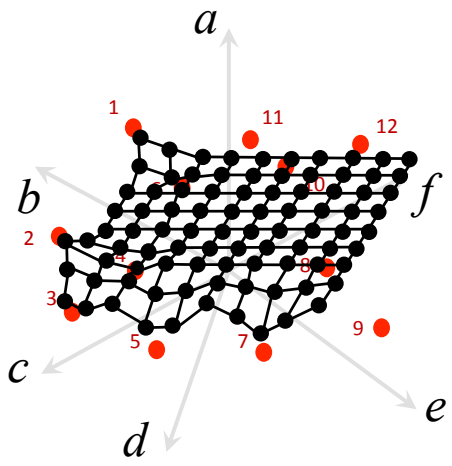
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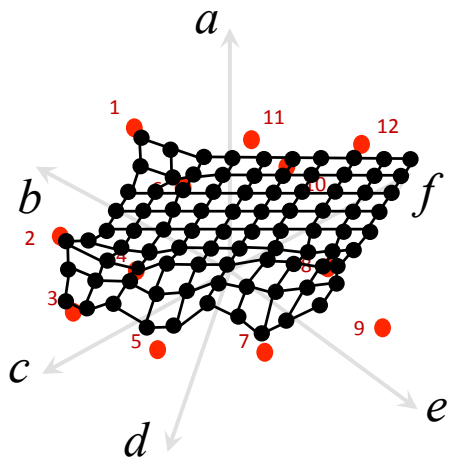
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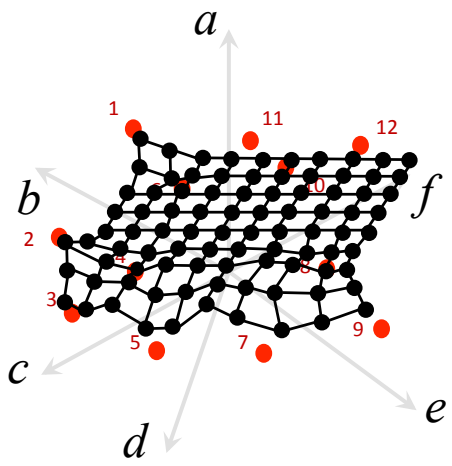
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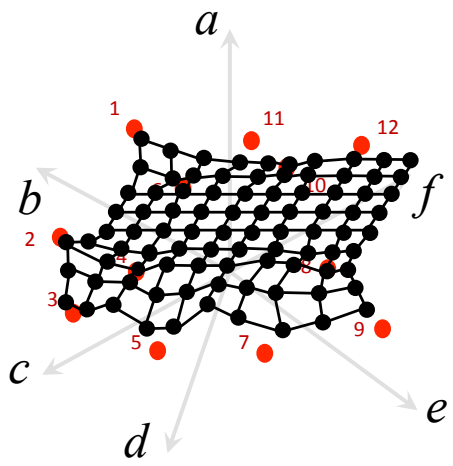
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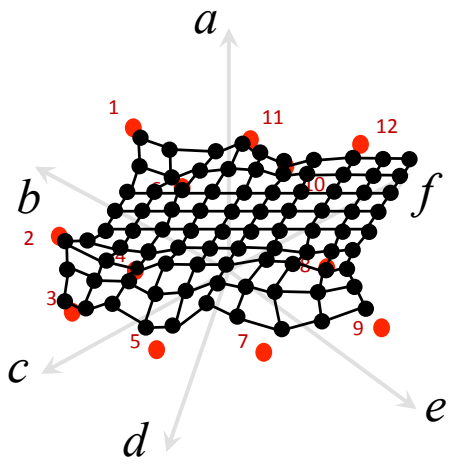
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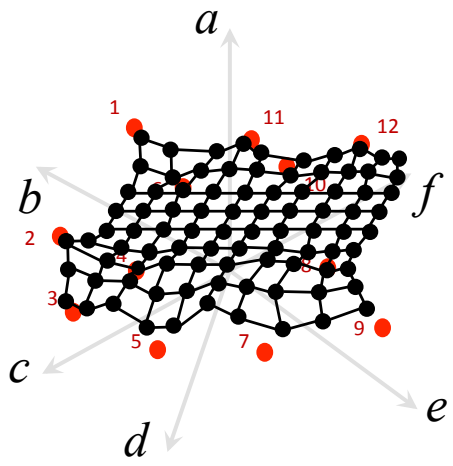
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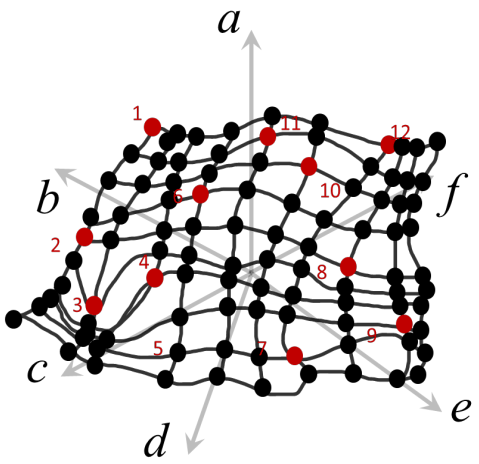
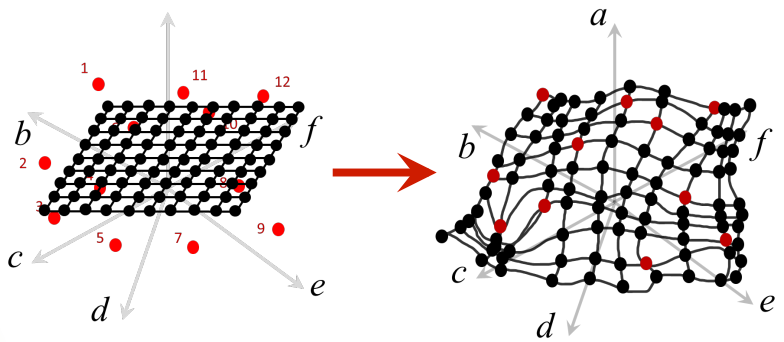
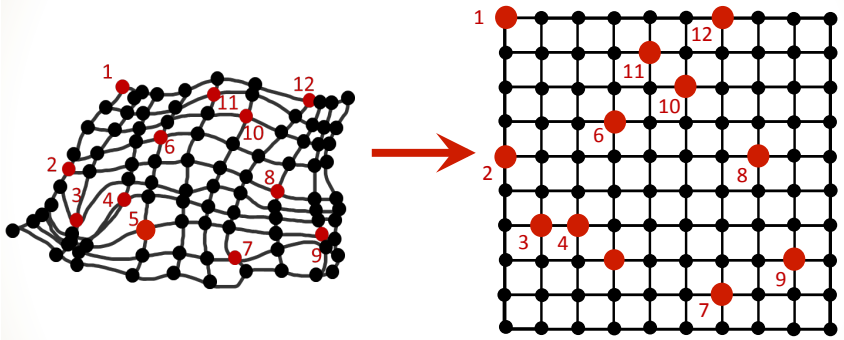


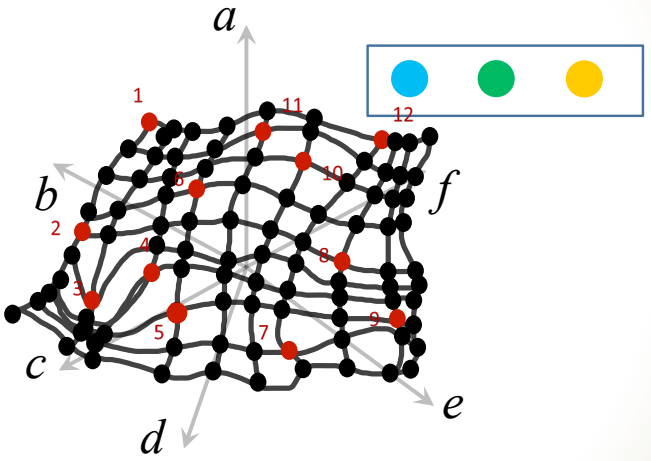
Deformation of the Meshes

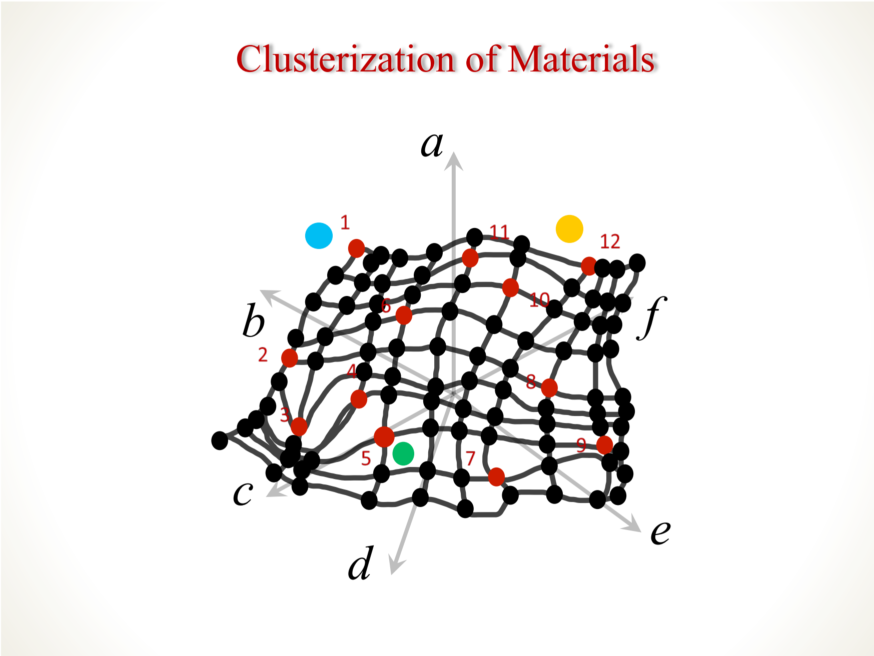


Dimensionality Reduction



Clusterization of Materials

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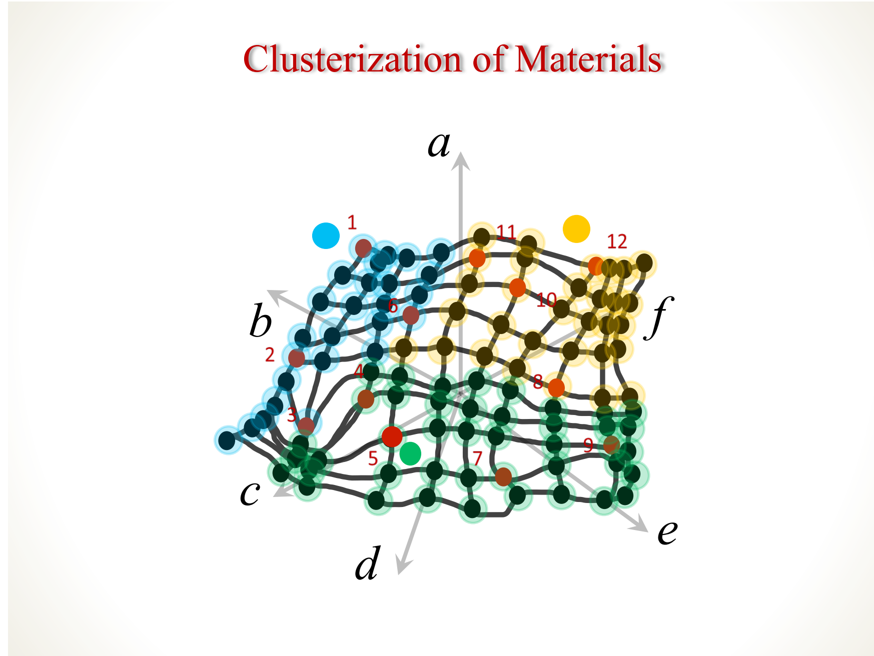
Clusterization of Materials
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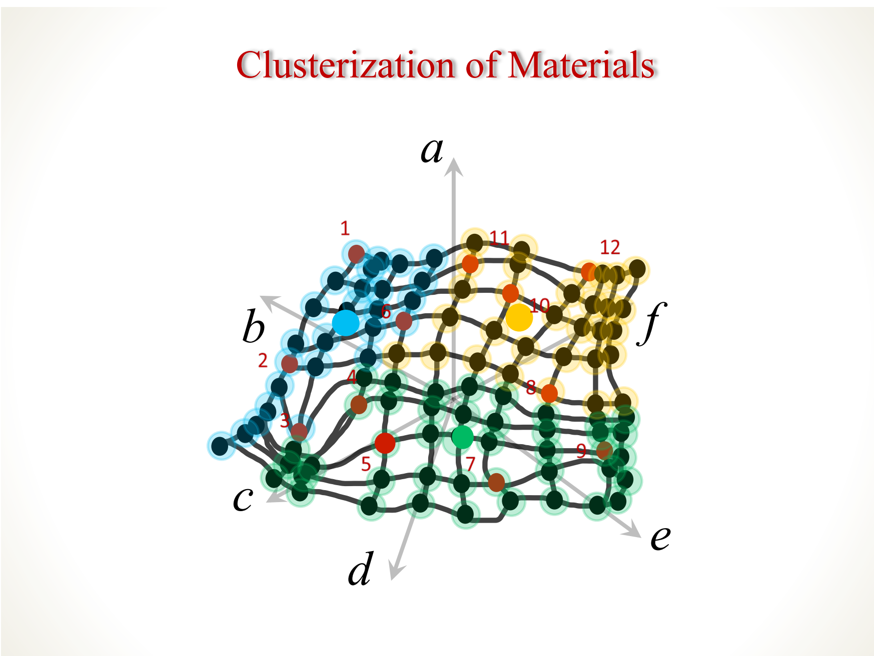
Clusterization of Materials
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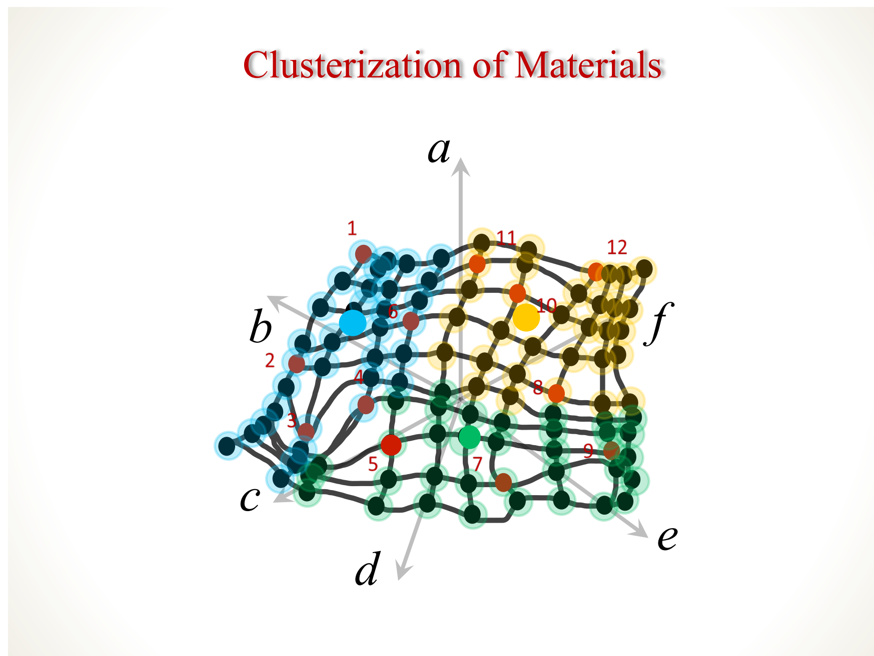
Clusterization of Materials
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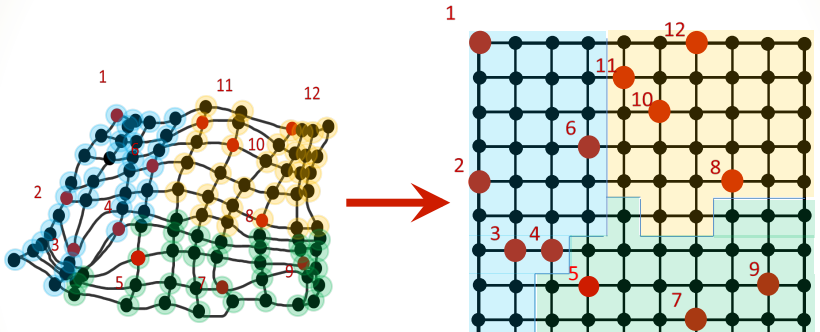
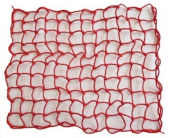
Catch and Release



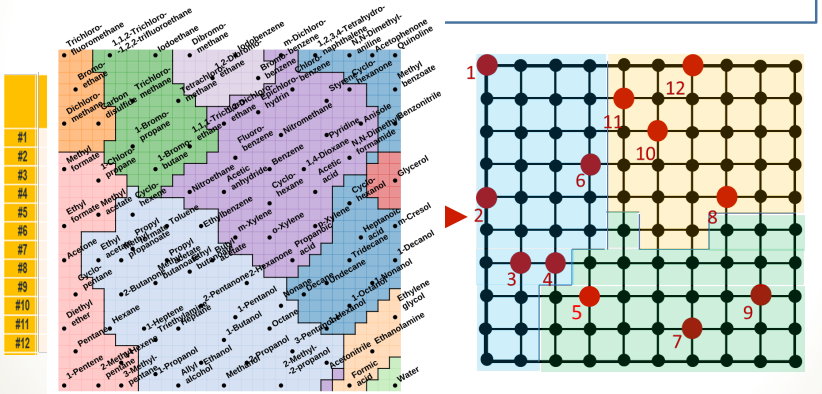


Release Elastic Energy !!

Dimensionality reduction

(High dimension data is projected onto low dimension.)

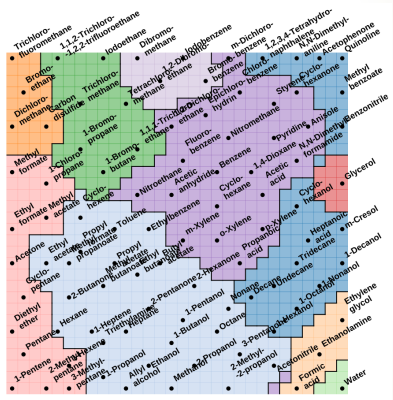
Culsterization of Materials



Application of SOM: Liquid Materials

molecular weight | melting point | boiling point | density | viscosity | heat capacity | vapor pressure | surface tension | thermal conductivity

Acetic acid	C2H4O2
Acetic anhydride	C4H6O3
Acetone	C3H6O
Acetonitrile	C2H3N
Acetophenone	C8H8O
Allyl alcohol	C3H6O
Anisole	C7H8O
Benzene	C6H6

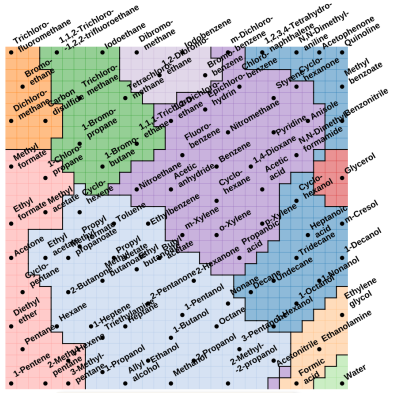


8 Properties

80 Materials

G.Kikugawa, et al (2018)

Application of SOM: Liquid Materials

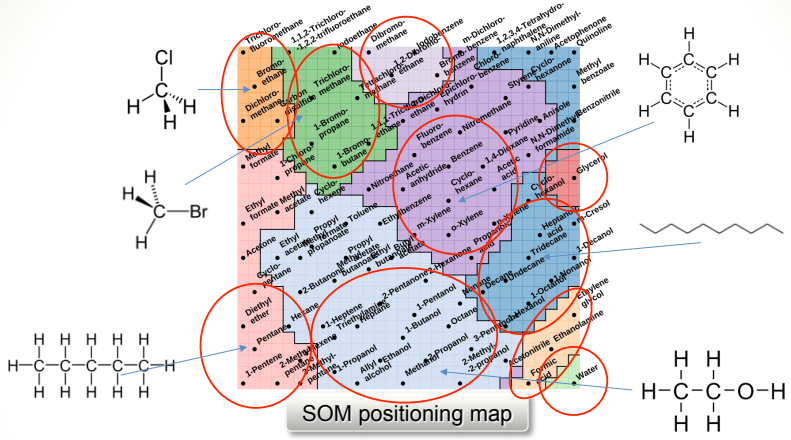


SOM positioning map

- Black solid lines denote the cluster boundaries determined by k-means method.

G.Kikugawa, et al (2018)

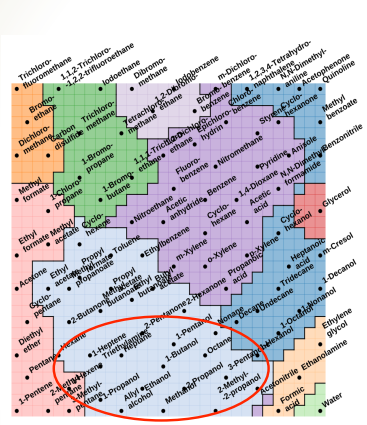
Application of SOM: Liquid Materials



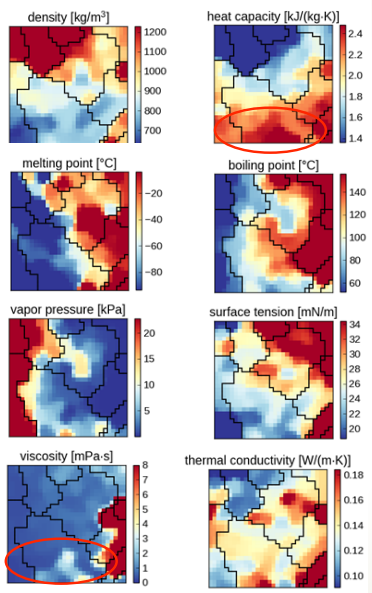
- Tested liquids are clustered by chemical compounds characterized with functional groups mostly well.

G.Kikugawa, et al (2018)

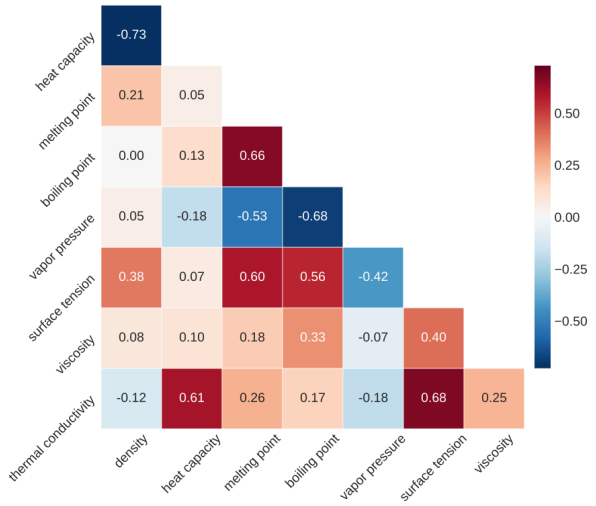
Application of SOM: Liquid Materials



Heat map of thermophysical properties

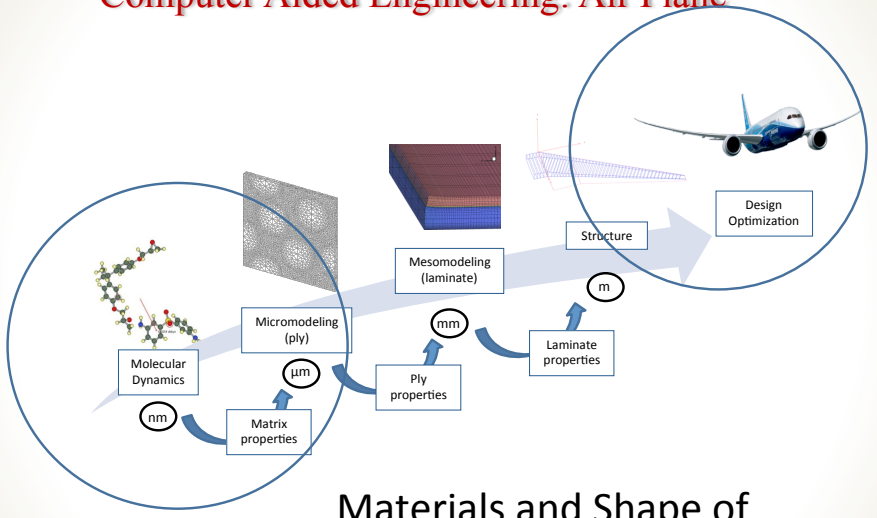


Application of SOM: Liquid Materials



- Overview of correlative relationship between two properties

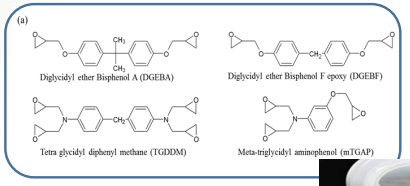
Computer Aided Engineering: Air Plane



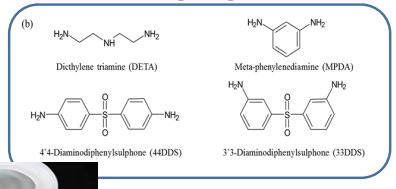
Materials and Shape of Air Plane Wing

Computer Aided Engineering: Air Plane

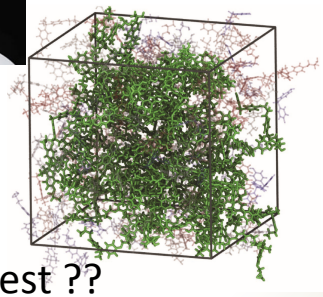
Base Resin



Curing Agent



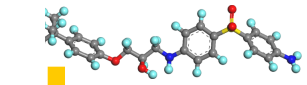
Mixing
Chemical Reaction

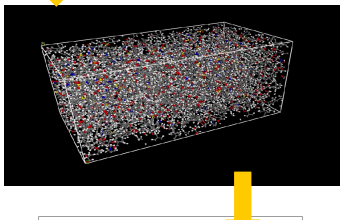


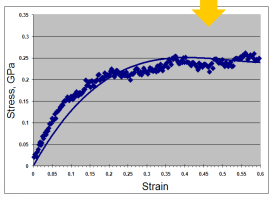
Cross-Linked!!

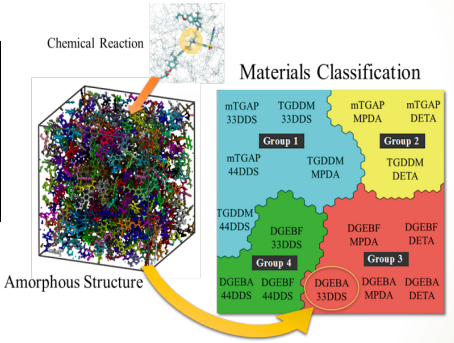
Which Combination is the best ??

Optimization of Thermosetting Resins





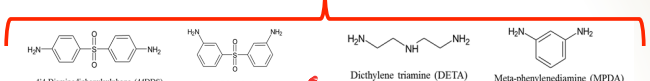




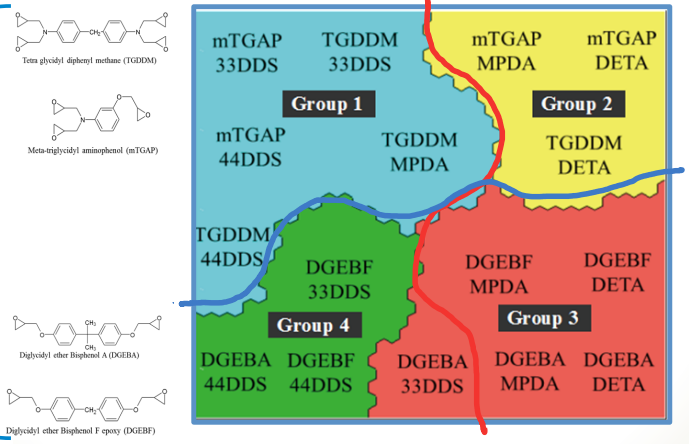
Y.Oya et al (2017)

Optimization of Thermosetting Resins

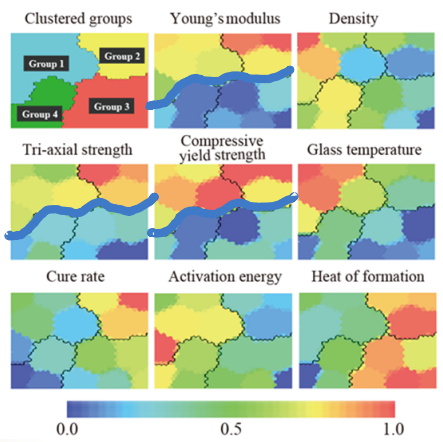
Curing Agents

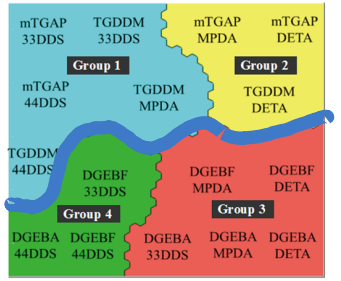


Base Resin



Optimization of Thermosetting Resins

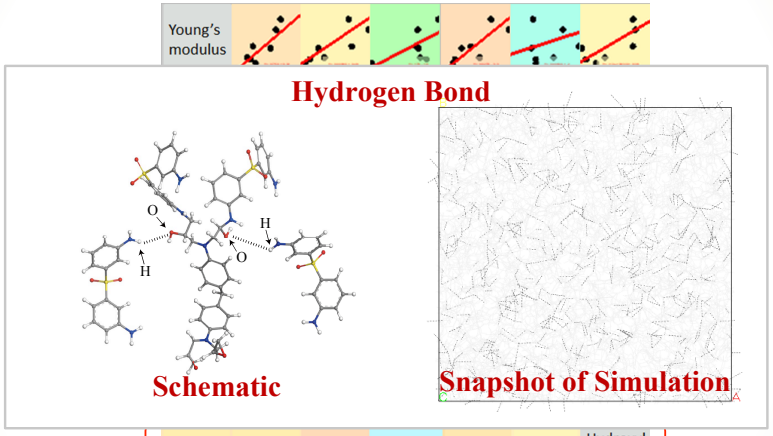




TGDDM/33DDS is candidate for the appropriate material

Materials in Group1, and Group 2 have higher Mechanical Properties

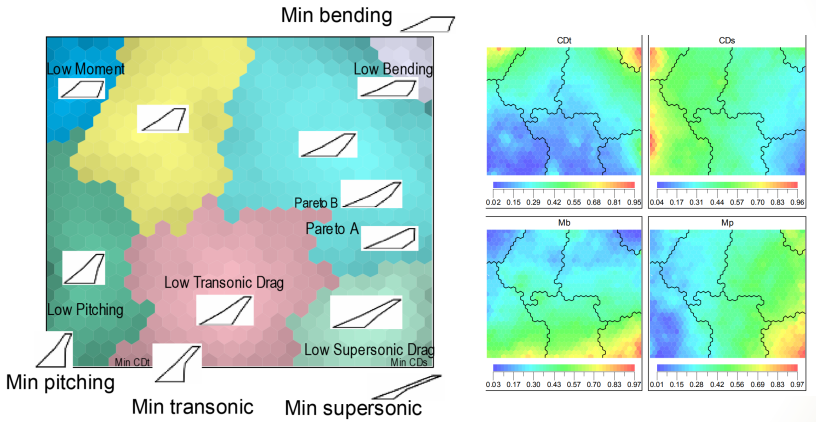
Optimization of Thermosetting Resins



0.78	0.79	0.91	0.17	0.82	0.74	Hydroxyl group /Volume

Density of Hydrogen Bond Affect Stiffness and Strength

Optimization of Wing Shape



Working on Project: Optimization of Ceramic

Thermoelectric Figure of Merit

$$FM = \frac{\sigma S^2}{\alpha}$$

Thermal shock

$$\mathrm{Rs} = \frac{\lambda \sigma_B}{\alpha E}$$

σ :electric conductivity
S :Seebeck coefficient
α :thermal conductivity

σ_B :mean bending strength
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E :elastic modulus

Working on Project: Optimization of Ceramic

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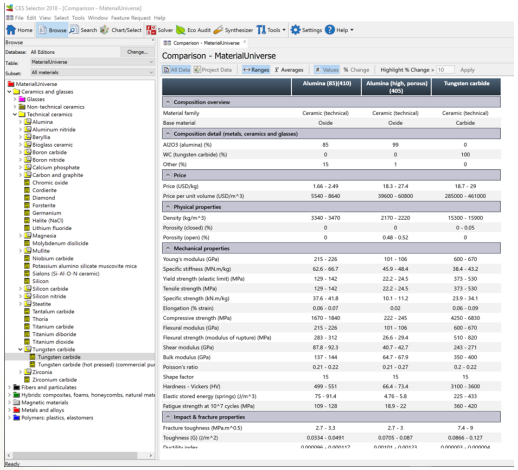
Working on Project: Optimization of Ceramic

GRANTA MATERIAL INTELLIGENCE

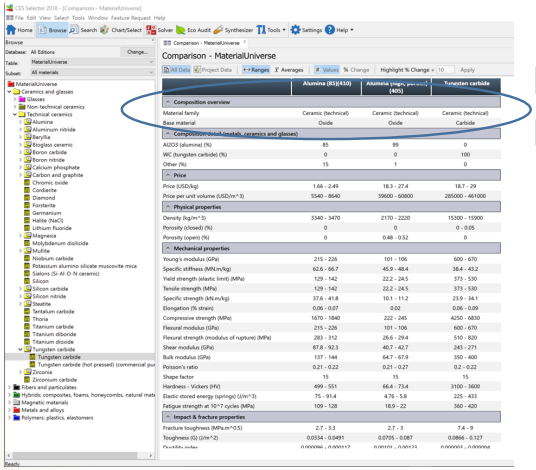


Huge Data Base

Over6000 Ceramics

Working on Project: Optimization of Ceramic

GRANTA MATERIAL INTELLIGENCE



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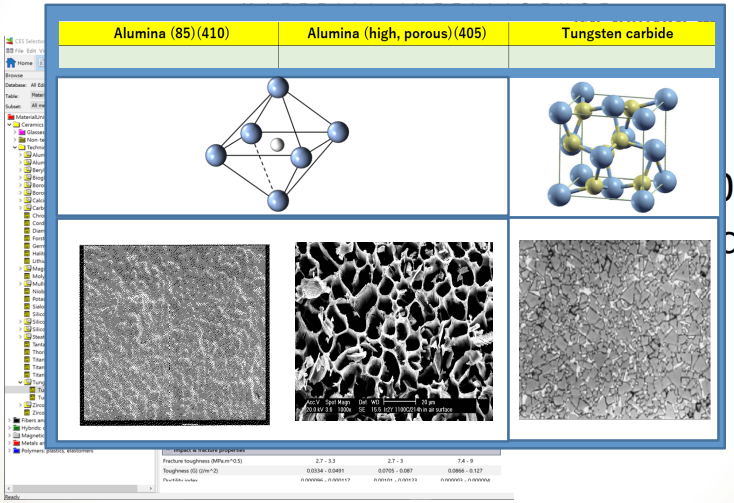
Working on Project: Optimization of Ceramic

GRANTA



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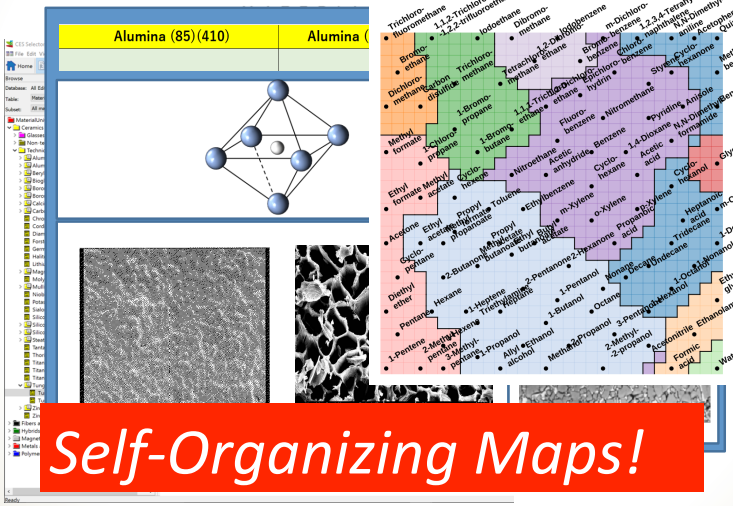
Working on Project: Optimization of Ceramic

GRANTA

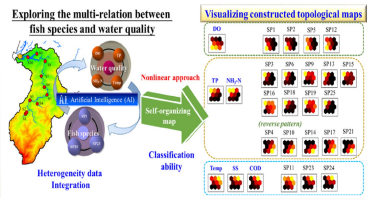


Self-Organizing Maps!

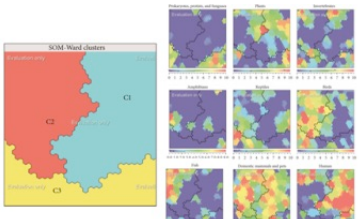
Conclusions

SOM has many advantages to grasp important features of the data through:

- Dimensionally Reduction
- Clustering
- 1 to 1 Relation between Materials and Properties
- Sorting Depends on Similarity



Wen-Ping Tsai [a], Shih-Pin Huang [b], Su-Ting Cheng [a], Kwang-Tsao Shao [b], Fi-John Chang [a,*] (2017)



Nurettin Yorek, Ilker Ugulu, and Halil Aydin (2016)