

Visual Alchemist: Visualization tool for data-driven materials science

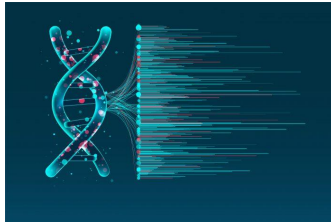
Shayan Monadjemi
Danni Liu
Bruktawit Amare



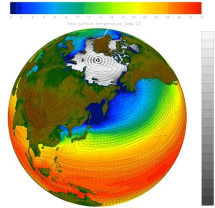
Data-driven research for scientific discovery

★ Data-driven science

Genomics



Climate science



Health care



Data-driven materials science

- ★ Existing material datasets
 - Analysing trends between compositions, structure and properties etc
- ★ Materials design and discovery
 - Identifying compositions, structures and synthesis conditions
- ★ Leads to accelerated discovery

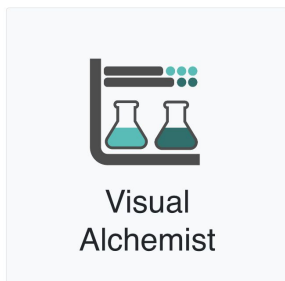
Problem

★ There is no interactive visualization tool

★ High-dimensionality of chemical compositions

1																		2																																													
H hydrogen 1.008																		He helium 4.0026																																													
3		4																10																																													
Li lithium 6.941		Be beryllium 9.0122																Ne neon 20.180																																													
11		12																18																																													
Na sodium 22.990		Mg magnesium 24.305																Ar argon 39.948																																													
3																		4		5		6		7		8		9		10		11		12		13		14		15		16		17		18																	
K potassium 39.098																		Ca calcium 40.078(4)		Sc scandium 44.956		Ti titanium 47.867		V vanadium 50.942		Cr chromium 51.996		Mn manganese 54.938		Fe iron 55.845(2)		Co cobalt 58.933		Ni nickel 58.693		Cu copper 63.546(3)		Zn zinc 65.38(2)		Ga gallium 69.723		Ge germanium 72.630(8)		As arsenic 74.922		Se selenium 78.971(8)		Br bromine 79.904		Kr krypton 83.798(2)													
37																		38		39		40		41		42		43		44		45		46		47		48		49		50		51		52		53		54													
Rb rubidium 85.468																		Sr strontium 87.62		Y yttrium 88.906		Zr zirconium 91.224(2)		Nb niobium 92.906		Mo molybdenum 95.95		Tc technetium 101.07(2)		Ru ruthenium 101.07(2)		Rh rhodium 102.91		Pd palladium 106.42		Ag silver 107.87		Cd cadmium 112.41		In indium 114.82		Sn tin 118.71		Sb antimony 121.76		Te tellurium 127.60(3)		I iodine 126.90		Xe xenon 131.29													
55																		56		57-71														72		73		74		75		76		77		78		79		80		81		82		83		84		85		86	
Cs cesium 132.91																		Ba barium 137.33		lanthanoids														Hf hafnium 178.49(2)		Ta tantalum 180.95		W tungsten 183.84		Re rhenium 186.21		Os osmium 190.23(3)		Ir iridium 192.22		Pt platinum 195.08		Au gold 196.97		Hg mercury 200.59		Tl thallium 204.38		Pb lead 207.2		Bi bismuth 208.98		Po polonium		At astatine		Rn radon	
87																		88		89-103														104		105		106		107		108		109		110		111		112		113		114		115		116		117		118	
Fr francium																		Ra radium		actinoids														Rf rutherfordium		Db dubnium		Sg seaborgium		Bh bohrium		Hs hassium		Mt meitnerium		Ds darmstadtium		Rg roentgenium		Cn copernicium		Nh nihonium		Fl flerovium		Mc moscovium		Lv livermorium		Ts tennessine		Og oganesson	
57																		58		59		60		61		62		63		64		65		66		67		68		69		70		71																			
La lanthanum 138.91																		Ce cerium 140.12		Pr praseodymium 140.91		Nd neodymium 144.24		Pm promethium		Sm samarium 150.36(2)		Eu europium 151.96		Gd gadolinium 157.25(3)		Tb terbium 158.93		Dy dysprosium 162.50		Ho holmium 164.93		Er erbium 167.26		Tm thulium 168.93		Yb ytterbium 173.05		Lu lutetium 174.97																			
89																		90		91		92		93		94		95		96		97		98		99		100		101		102		103																			
Ac actinium																		Th thorium 232.04		Pa protactinium 231.04		U uranium 238.03		Np neptunium		Pu plutonium		Am americium		Cm curium		Bk berkelium		Cf californium		Es einsteinium		Fm fermium		Md mendelevium		No nobelium		Lr lawrencium																			

Visual Alchemist

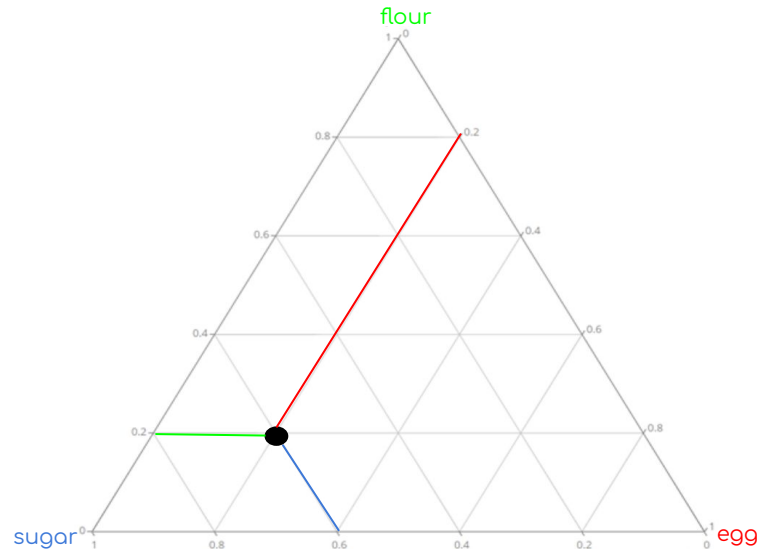


Interactivity

- ★ 2 visualization techniques
 - Ternary plots
 - Parallel coordinate planes

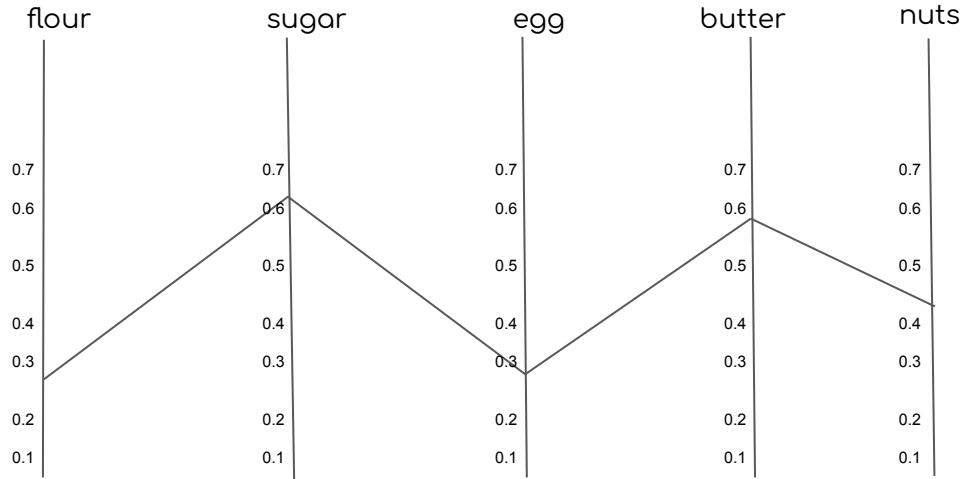
Ternary Plots

★ Three elements

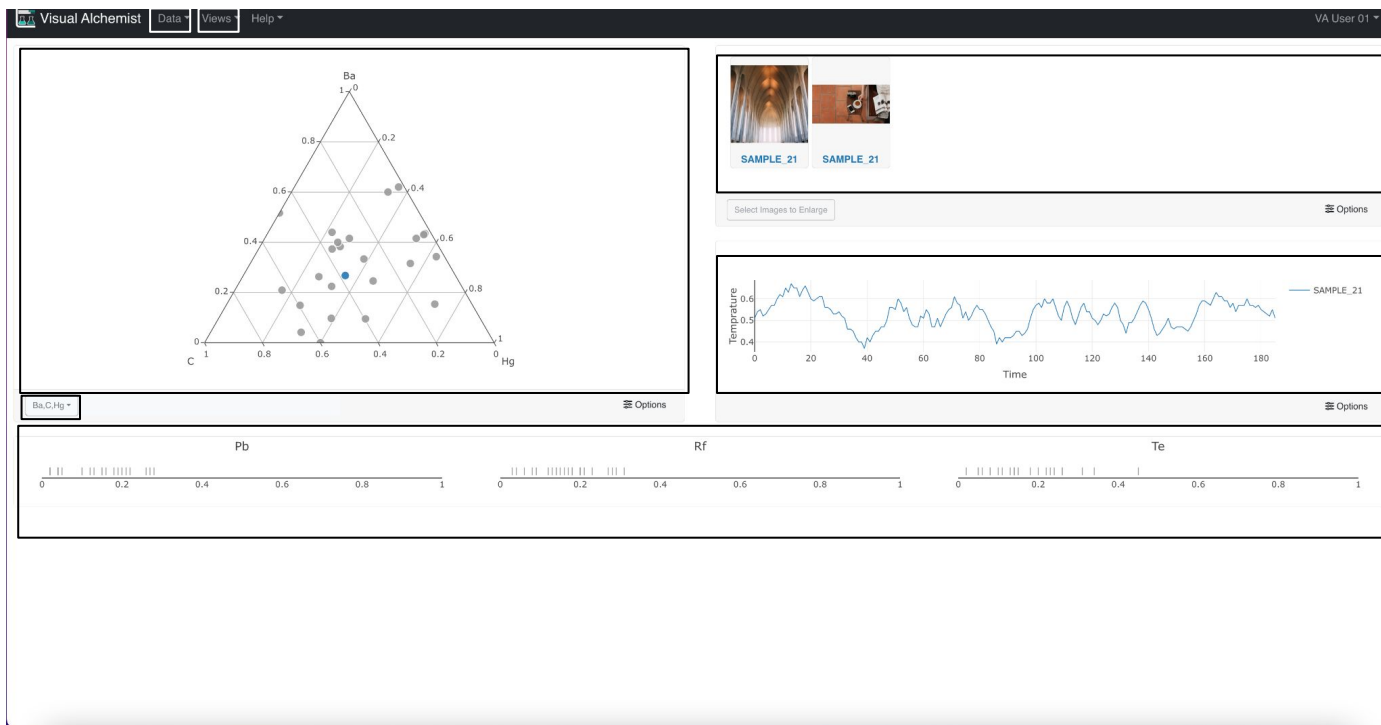


Parallel Coordinate Planes

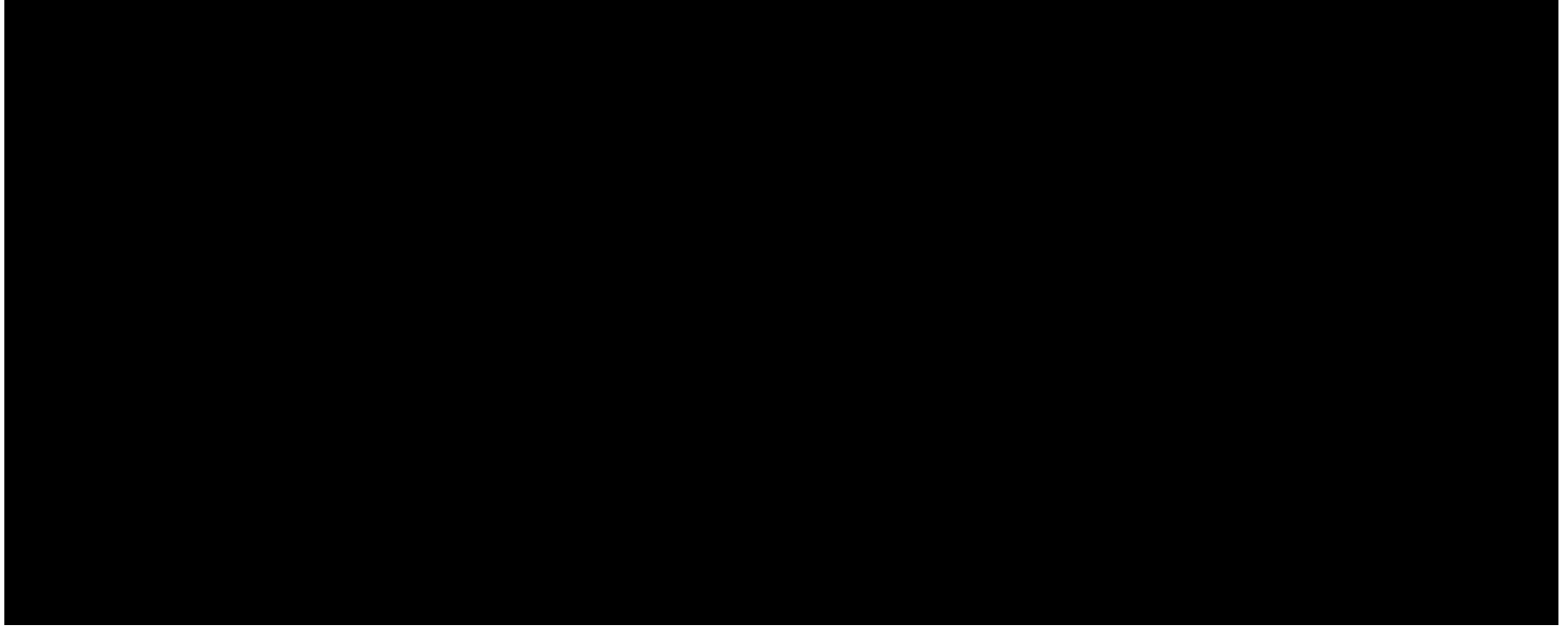
★ Many elements



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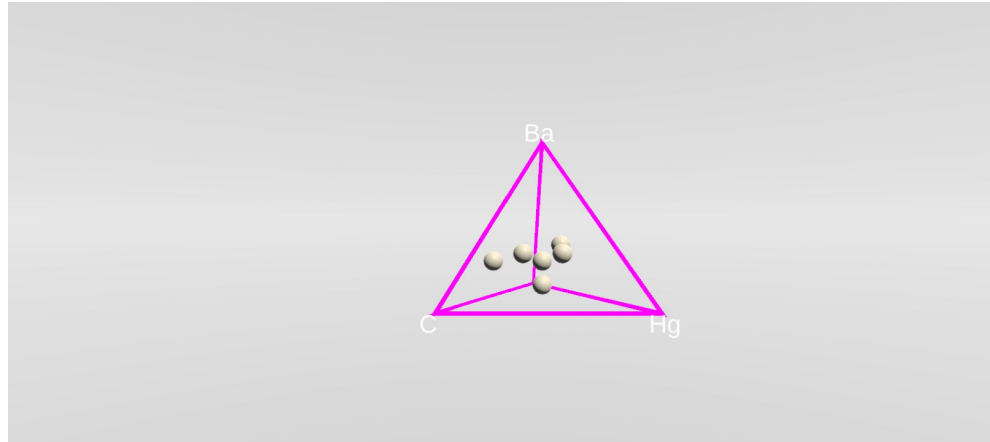


Demo



Future directions

- ★ 3D data visualization



- ★ User study

Post-baccalaureate research internship

- ★ Research experience
- ★ Graduate school



Prof. Alvitta Ottley



Shayan Monadjemi



THANK YOU!