PerTabVIS

CPSC 533C 2011/W1 Project Proposal

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1. Abstract

This project proposal presents an application named PerTabVIS, a tool using a visualization approach to explore Periodic Table for general users. The purpose of PerTabVIS is to provide people with a visualized and interactive approach to learn element properties and compare the relationship between them, and to show a regular pattern for certain properties such as PH value (pondus hydrogenii value), metallicity, boiling point and so on.

2. Background and Previous Work

Substances around us constitute such a miracle and splendid world. If exploring deeper in what we see every day, we will know these colorful and variant substances consist of different elements as a most intrinsic combination. Scientists recognized there must be some laws to organize them together and corresponding disciplines to distinguish them. Thus, [Dmitri Mendeleev, 1869]^[1] presented his assumption of pattern of elements, which is the prototype of Periodic Table we see nowadays, like in Figure 1. In this project, I will still use the traditional Periodic Table in Figure 1 although there are lots of modern versions.

			1 H drogen	– atomic numbe – symbol	r atomic n left-hand second is having the same colu	umber, startir corner and cor by the number same number mn. Since the	ig with hydrog ntinuing in asc er of electron of electrons in number of ele	I elements in tw en (atomic num ending order fi s in the outer the outermost ctrons in the o	ber = 1) in th rom left to right most shell. E shell are place utermost shell	e upper ht. The lements d in the in large			Metals	Nonmetal	s Noble gases			
	Group 1a	1.	00794	 atomic weight (or mass numl of most stable isotope if in 	er column ha This a	we similar cher trangement of	nical properties the elements w	if an element, , ras devised by I r known were d	Omitri Mende	leev in								Group 0
Period 1	Hydrogen 1.00794	Group 2a		parentheses)	elements filled in, r has been i	the overall logic of the table. Mendelever allowed space for undiscovered elements whose existence he predicted. This space has since been partly filed in most received by the addition of elements 104–112. Element 112 has been isolated experimentally but not yet officially named. The fanthanise series (elements 57–71) and the actinide series								Group 4a	Group 5a	Group 6a	Group 7a	Helium 4.0026
Period 2	Lithium 6.941	Be Beryllium 9.0122				They are pla		elements with main body of					Boron 10.811	Carbon 12.011	Nitrogen 14.0067	Oxygen 15.9994	P F Fluorine 18.9984	10 Neon 20.183
Period 3	Na Sodium 22.9898	Magnesium 24.305	Group 3b	Group 4b	Group 5b	Group 6b	Group 7b	Group 8	Group 8	Group 8	Group 1b	Group 2b	Aluminum 26.9815	Silicon 28.086	Phosphorus 30.9738	16 S Sulfur 32.066	Chlorine 35.453	Argon 39.948
Period 4	Potassium 39.098	Calcium 40.08	Scandium 44.956	Titanium 47.87	Vanadium 50.942	Chromium 51.996	Manganese 54.9380	Fe Iron 55.845	Cobalt 58.9332	Nickel 58.69	Copper 63.546	2n Zn 55.39	Gallium 69.72	Germanium 72.61	33 As Arsenic 74.9216	Selenium 78.96	Bromine 79.904	Krypton 83.80
Period 5	Rubidium 85.47	Sr Sr strontium 87.62	Yttrium 88.906	Zr Zirconium 91.22	Niobium 92.906	Molybdenum 95.94	Tc Tc Technetium (98)	Ru Ru 101.07	Rhodium 102.905	Palladium	47 Ag Silver 107.868	Cadmium	49 In Indium 114.82	50 Sn 118.71	Sb Antimony 121.76	Tellurium	53 lodine 126.9045	54 Xenon 131.29
Period 6	55 CS Cesium 132.905	Barium 137.33	57–71* Lanthanides	Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	Rhenium 186.2	76 OS Osmium 190.2	77 Ir Iridium 192.2	Platinum 195.08	79 Au Gold 196.967	Hg Mercury 200.59	TI Thallium 204.38	Pb Lead 207.2	83 Bi Bismuth 208.98	Polonium (210)	Astatine (210)	Radon (222)
Period 7	Francium (223)	Radium (226)	89–103** Actinides	Rutherfordium (261)	Dubnium (262)	Db Sg Bh Hs Mt Ds Rg						† Until official names are given to new elements, names based on a Latin translation the atomic number are used; e.g. ununbium (Latin unus 11 + unus 11 + bi- 22) for element 112.						
	*LANTH	ANIDES	Lanthanum	58 Cerium 140.12	Praseodymium	Neodymium 144,24	Promethium	52 Sm 5amarium 150.36	Europium	Gadolinium	Tb Terbium 158.925	Dysprosium 162,50	67 Ho Holmium 164.930	68 Er Erbium 167.26	69 Tm Thulium 168.934	Ytterbium 173.04	71 Lu Lutetium 174.97	
	**ACTIN	IIDES	Actinium (227)	90 Th Thorium 232.038	Protactinium 231.036	92 U Uranium 238.03	93 Np Neptunium (237)	94 Pu Plutonium (244)	Americium (243)	Curium (247)	Brkelium (247)	Californium (251)	99 ES Einsteinium (252)	Fermium (257)	Mendelevium (258)	Nobelium (259)	Lawrencium (262)	
	ALPHABET	ICAL TABLE			tomic		Atomic		Atomic	-		Atomic		Atomic		Atomic		A
	Actinium Aluminum Americium	Atom ymbol Numb Ac 89 Al 13 Am 95 Sb 51 Ar 18 As 33 At 85 Ba 56 Bk 97 Be 4		Symbol N Cd Ca	tomic umber Elemen 48 Einsteir 20 Elemen 98 Erbium 6 Europiu 58 Fermiur 55 Fluorin 17 Franciu 24 Gadder 27 Gallur 29 Germar	sium Es t 112 – m Eu n Fra e F m Fr sium Gd a Gal	Number E 99 9 112 9 68 0 63 0 100 0 9 0 87 X 64 L 31 L	idium I odine idium I on F iypton I	bol Number lo 67 1 1 n 49 I 53 r 77 e 26 tr 36 a 57 s 103	F Element Meitnerium Mendeleviu Mercury Molybdenuu Neodymium Neodymium Neptunium Nickel Niobium Nibium	Symbol M Mt m Md Hg n Mo	Number Elem 109 Phose 101 Flatin 80 Pluton 42 Polon 60 Potas 10 Prase 93 Promo	Rorus P um Pt nium Pu um Po sum K sodymium Pr ethium Pm ttinium Pa m Ra	Number E 15 R 78 R 94 S 84 S 19 S 59 S 61 S 91 S 88 S	licon : Iver / odium : I	abol Number tu 44 til 104 tm 62 ic 21 ig 106 ie 34 5i 14 ig 47		Symbol N Tb Ti Th Tm Sn Ti W U U V Xe
	Bismuth Bohrium Boron Bromine	Bi 83 Bh 107 B 5 Br 35	Curium Darmstadtie Dubnium Dysprosium	Cm Ds Db	96 Gold 110 Hafniur 105 Hassiur 66 Helium	Au n Hf n Hs	79 L 72 L 108 M	ithium 1	i 3 u 71 lg 12	Nobelium Osmium Oxygen Palladium	NO OS O PO	102 Rheni 76 Rhodi	um Re um Rh Igenium Rg	75 Si 45 Ti 111 Ti	ulfur antalum 1 echnetium 1	5 16 a 73 c 43 e 52	Ytterbium Ytteiam Zinc Zirconium	Yb Y Zn Zr

However, whether with any relative chemistry background or not, it is hard to figure out any relationship at first sight from Periodic Table shown above. Thus, if we could design a visualized tool to show the potential relationship in a direct way, it might be very helpful for people to learn and grasp elements, or even discover new elements.

Realizing this problem, during the past few decades, developers have developed kinds of visualized tool to better reveal Periodic Table. For instance, [Christopher Ahlberg 1992]^[2] devised a *dynamics queries* to search and show the elements in the table. More implementations are used in the industrial and educational field. There are lots of applications for Periodic Table available on the website. However, the existed tools all have pros and cons. Some of them focus on the history and the background of element. *How does an element look like? Who, when and where discover it?* i.e., *The visual Elements Periodic Table*^[3]. In addition, some others only care about each element itself but ignore the relation between elements, i.e. *David's Whizzy Periodic Table*^[4] & *Periodic Table Live*^[5]. Some other implementations like *The Pictorial Periodic Table*^[6], *Periodic Table of the Elements*^[7] and *Interactives: Periodic Table*^[8] reveal some relations but don't allow users to select elements used to compare according to own willing. On the other hand, some advanced tools do reveal complex relationships but it seems more like to design for an expert but not for general users, i.e., *elements*^[9] on the *Improvise* website.

Thus, I want to develop a visualization tool which can well show both information of each element and connections between different properties. And above all, this tool is toward general users.

The following sections of this proposal will be organized as this way. Section 3 describes the problem domain, task and dataset used and then section 4 is a further illustration combined with personal experience. The scenario of use is exemplified in section 5. In the next two following sections 6 and 7, possible solution and implementation approach will be proposed and described, respectively. At last, section 8 lists my project schedule.

3. Domain, Task and Dataset

PerTabVIS is intended to reveal the relationship between elements in visualization way. The domain and task of this application is naturally to provide a visualized and interactive approach for general users who is in or interested in chemical field. The dataset can be easily found on the website such as Wikipedia. The data I will use here is mainly from one example named *elements*^[9] on the *Improvise* website. This dataset includes such amount of basic information about elements like isotope, acidity and alkaline, radius of atom, boil point, spatial structure that it is enough for general users.

4. Personal Experience

When in senior school, I once learned Chemistry as a compulsory course. The Periodic Table of Elements is one of most basic and important knowledge for students who first stepping into chemical field. But unfortunately, most of students might be confused by the complex relationship between elements. What I did at that time is just to remember all of them in heart. After realizing that visualization is a powerful approach to reveal the numerical and abstract concept visually, I think I can make some efforts to help senior students easily grasp Periodic Table. And with regard of some chemical background, I have a concept what general users interest in.

5. Scenario of Use

Considering PerTabVIS is for general users such as students in senior school, the scenario of use should focus on the basic concept in the Periodic Table. Suppose Austin is a senior school student. A typical scenario of use for PerTabVIS is that midterm will come soon, but Austin still has no idea about how Na exists and looks like in the real world, as an elementary

substance or compound? Then he right clicks Na element by using mouse. PerTabVIS then shows a menu besides the element including many options. Austin finds there is an option called "look like". Then he clicks it and PerTabVIS shows some most common existing states of Na in the world and the spatial structure. Then Austin knows Na usually exists as a compound such as NaCl.

Another likely scenario of use for PerTabVIS is to compare multiple properties between elements. User selects elements by clicking them in the table and then selects which properties to compare. PerTabVIS will show the outcome in a most popular way. That is to say, display relies on physiological perception. In addition, user can also choose own preferred display method. For example, Austin wants to compare the PH value for some elements. Then he selects several elements in the Periodic Table by combination of 'ctrl' button and left-click and chooses "PH value". PerTabVIS then shows the PH value in other window from low to high, from acidity to alkaline, with a rainbow color encoding. Here, PerTabVIS also provides Austin with an option to see the PH value numerical way or histogram way. Besides, Austin also wants to see the relationship between boiling point and radius, namely multiple properties comparison. Then he selects "radius" and "boiling point" in the option menu and gets outcome with line chart in a 2D coordinate frame.

6. Proposed Solution

The constant number of elements in Periodic Table indicates limited size of dataset. So the abstraction of data should be focused on category. Which elements are metal? Which group has similar property? Such kind of questions should be well devised. Furthermore, one element might have lots of attributes, such as proton number, isotope. All of its attributes should be bounded together as member variable of this element object. So I derive the general hierarchy of data seen in Figure 2.

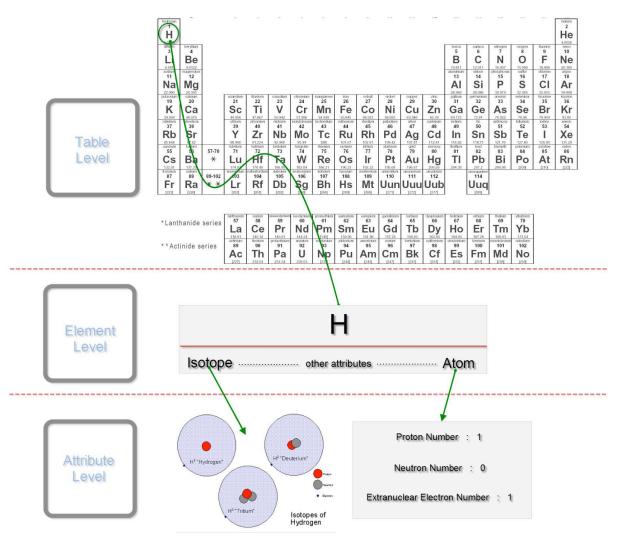


Figure 2 Data Hierarchy

PerTabVIS is a user-driven platform, which means PerTabVIS displays whatever user is willing to see, unless the meta-data is in the dataset. This feature might be the most different part compared with current tools which I mentioned above. To reach this purpose, a well-designed encoding system and a user-oriented interface can't be more significant. For the encoding method, I plan to use color, chart and size as mainly encoding approach. Color has lots of usage in PerTabVIS. For example, each row (period) and each column (group or family) will be easily recognized by different color. The scale of PH value can also be perceived easily in terms of saturation. As for the spatial structure for a compound, different element used to organize it can be well distinguished by different color. Chart is also a powerful method to reveal potential relationship of compared properties. For example, when measuring connection between boiling point and radius, a line chart might be very useful. When comparing radius, using circle to indicate relative size will be also very helpful.

As for interface techniques, multiple view approach does first come into my mind. For example, using linked view allow user to see different attributes at the same time. If a view displays mass of elements and the other view shows the density, user can choose one subregion from mass view and the corresponding density will be automatically highlighted in another view. Another technique worth to use is dynamic interaction. Suddenly popping out the outcome is suffering to the bad user experience. One more thing about interface is that about friendly UI. First, a friendly UI must be easy to understand. Here, I mean user must easily recognize the property he queries from mass of data. Second, a good interaction must be easy to handle. That is to say, user with little computer experience should also control it easily.

7. Implementation Approach

I prefer to use *HTML* combining with *D3.* $Js^{[10]}$ as my implementation toolkit. *HTML* is well used nowadays. And *D3.js* is a brand-new toolkit released on 2011 given strengthens of object-oriented model and dynamic interface.

8. Mile Stones

Deadline	Event Must be Done
Nov. 10	Categorize dataset and Abstract task
Nov. 15	Design interface and Draw an elementary frame
Nov. 20	Learn <i>D3 js</i> and relative knowledge
Nov. 30	Implement PerTabVIS
Dec. 05	Debug
Dec. 10	Complete project write-up

Reference

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- 3. The visual Elements Periodic Table, http://www.rsc.org/chemsoc/visualelements/pages/pertable_fla.htm
- 4. David's Whizzy Periodic Table, http://www.colorado.edu/physics/2000/applets/a2.html
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- 10. D3. js, http://mbostock.github.com/d3/