

PerTabVIS: A Visualized Tool for Periodic Table

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ABSTRACT

This paper introduces a new visualized tool for periodic table, named PerTabVIS. Compared with other related work, PerTabVIS can compare multi-properties and explore elements distribution according to user selection. The goal of this application is to provide both students in senior class and others majoring in Chemistry with a general web-based application to learn the periodic table and explore relationships between different properties.

KEYWORDS: Periodic table, elements, property comparison, user selection, elements distribution, interaction

1 INTRODUCTION

Periodic Table (as shown in Figure 1), first proposed by Dmitri Mendeleev [1] in 1869, is a tabular display of 118 known chemical elements organized by selected properties according to their atomic structure. Since the periodic table contains a wide variety of information such as element symbols, atomic number, and atomic mass, it is a very useful tool for students learning Chemistry. Besides, benefiting from the good property of periodic table to accurately predict the abilities of various elements, Chemists or related researchers make use of it as a useful framework to classify, systematize, and compare many different forms of chemical elements behaviour, or even discover new elements. Before going further, it will be helpful to clarify some basic terminologies used in Chemistry, which is also used in this paper. The purpose of it is to unify the related concepts and make up some necessary knowledge to those who have little chemical background.

- *Atomic number:* The number of protons found in the nucleus of an atom
- *Atomic symbol:* A 1- or 2-letter internationally agreed code for a chemical element, usually derived from the name of the element, often in Latin. Only the first letter is capitalised.
- *Electron Shells:* An orbit followed by electrons around an atom's nucleus.
- *Electrons per Shell:* Electron numbers on each electron shell.
- *Melting Point:* Temperature at which it changes state from solid to liquid.
- *Boiling Point:* Temperature at which it can change its state from a liquid to a gas.
- *Critical Point:* The conditions like temperature, pressure and sometimes composition at which a phase boundary ceases to exist.
- *Heat of Fusion:* The temperature at which one mole of a

substance changes states from a solid to a liquid resulting from heating.

- *Heat of Vaporization:* The energy required to transform a given quantity of a substance into a gas at a given pressure.
- *Period:* Each row in the periodic table is called a period. Elements of the same period have the same number of electron shells.
- *Family or Group:* Each column in the periodic table is called a period. Elements of the same family have similar properties.

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(307)	174 Uuq (309)	175 Uuq (311)	176 Uuq (313)	177 Uuq (315)	178 Uuq (317)	179 Uuq (319)	180 Uuq (321)	181 Uuq (323)	182 Uuq (325)	183 Uuq (327)	184 Uuq (329)	185 Uuq (331)	186 Uuq (333)	187 Uuq (335)	188 Uuq (337)	189 Uuq (339)	190 Uuq (341)	191 Uuq (343)	192 Uuq (345)	193 Uuq (347)	194 Uuq (349)	195 Uuq (351)	196 Uuq (353)	197 Uuq (355)	198 Uuq (357)	199 Uuq (359)	200 Uuq (361)	201 Uuq (363)	202 Uuq (365)	203 Uuq (367)	204 Uuq (369)	205 Uuq (371)	206 Uuq (373)	207 Uuq (375)	208 Uuq (377)	209 Uuq (379)	210 Uuq (381)	211 Uuq (383)	212 Uuq (385)	213 Uuq (387)	214 Uuq (389)	215 Uuq (391)	216 Uuq (393)	217 Uuq (395)	218 Uuq (397)	219 Uuq (399)	220 Uuq (401)	221 Uuq (403)	222 Uuq (405)	223 Uuq (407)	224 Uuq (409)	225 Uuq (411)	226 Uuq (413)	227 Uuq (415)	228 Uuq (417)	229 Uuq (419)	230 Uuq (421)	231 Uuq (423)	232 Uuq (425)	233 Uuq (427)	234 Uuq (429)	235 Uuq (431)	236 Uuq (433)	237 Uuq (435)	238 Uuq (437)	239 Uuq (439)	240 Uuq (441)	241 Uuq (443)	242 Uuq (445)	243 Uuq (447)	244 Uuq (449)	245 Uuq (451)	246 Uuq (453)	247 Uuq (455)	248 Uuq (457)	249 Uuq (459)	250 Uuq (461)	251 Uuq (463)	252 Uuq (465)	253 Uuq (467)	254 Uuq (469)	255 Uuq (471)	256 Uuq (473)	257 Uuq (475)	258 Uuq (477)	259 Uuq (479)	260 Uuq (481)	261 Uuq (483)	262 Uuq (485)	263 Uuq (487)	264 Uuq (489)	265 Uuq (491)	266 Uuq (493)	267 Uuq (495)	268 Uuq (497)	269 Uuq (499)	270 Uuq (501)	271 Uuq (503)	272 Uuq (505)	273 Uuq (507)	274 Uuq (509)	275 Uuq (511)	276 Uuq (513)	277 Uuq (515)	278 Uuq (517)	279 Uuq (519)	280 Uuq (521)	281 Uuq (523)	282 Uuq (525)	283 Uuq (527)	284 Uuq (529)	285 Uuq (531)	286 Uuq (533)	287 Uuq (535)	288 Uuq (537)	289 Uuq (539)	290 Uuq (541)	291 Uuq (543)	292 Uuq (545)	293 Uuq (547)	294 Uuq (549)	295 Uuq (551)	296 Uuq (553)	297 Uuq (555)	298 Uuq (557)	299 Uuq (559)	300 Uuq (561)	301 Uuq (563)	302 Uuq (565)	303 Uuq (567)	304 Uuq (569)	305 Uuq (571)	306 Uuq (573)	307 Uuq (575)	308 Uuq (577)	309 Uuq (579)	310 Uuq (581)	311 Uuq (583)	312 Uuq (585)	313 Uuq (587)	314 Uuq (589)	315 Uuq 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(733)	387 Uuq (735)	388 Uuq (737)	389 Uuq (739)	390 Uuq (741)	391 Uuq (743)	392 Uuq (745)	393 Uuq (747)	394 Uuq (749)	395 Uuq (751)	396 Uuq (753)	397 Uuq (755)	398 Uuq (757)	399 Uuq (759)	400 Uuq (761)	401 Uuq (763)	402 Uuq (765)	403 Uuq (767)	404 Uuq (769)	405 Uuq (771)	406 Uuq (773)	407 Uuq (775)	408 Uuq (777)	409 Uuq (779)	410 Uuq (781)	411 Uuq (783)	412 Uuq (785)	413 Uuq (787)	414 Uuq (789)	415 Uuq (791)	416 Uuq (793)	417 Uuq (795)	418 Uuq (797)	419 Uuq (799)	420 Uuq (801)	421 Uuq (803)	422 Uuq (805)	423 Uuq (807)	424 Uuq (809)	425 Uuq (811)	426 Uuq (813)	427 Uuq (815)	428 Uuq (817)	429 Uuq (819)	430 Uuq (821)	431 Uuq (823)	432 Uuq (825)	433 Uuq (827)	434 Uuq (829)	435 Uuq (831)	436 Uuq (833)	437 Uuq (835)	438 Uuq (837)	439 Uuq (839)	440 Uuq (841)	441 Uuq (843)	442 Uuq (845)	443 Uuq (847)	444 Uuq (849)	445 Uuq (851)	446 Uuq (853)	447 Uuq (855)	448 Uuq (857)	449 Uuq (859)	450 Uuq (861)	451 Uuq (863)	452 Uuq (865)	453 Uuq (867)	454 Uuq (869)	455 Uuq (871)	456 Uuq (873)	457 Uuq 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Uuq (1017)	529 Uuq (1019)	530 Uuq (1021)	531 Uuq (1023)	532 Uuq (1025)	533 Uuq (1027)	534 Uuq (1029)	535 Uuq (1031)	536 Uuq (1033)	537 Uuq (1035)	538 Uuq (1037)	539 Uuq (1039)	540 Uuq (1041)	541 Uuq (1043)	542 Uuq (1045)	543 Uuq (1047)	544 Uuq (1049)	545 Uuq (1051)	546 Uuq (1053)	547 Uuq (1055)	548 Uuq (1057)	549 Uuq (1059)	550 Uuq (1061)	551 Uuq (1063)	552 Uuq (1065)	553 Uuq (1067)	554 Uuq (1069)	555 Uuq (1071)	556 Uuq (1073)	557 Uuq (1075)	558 Uuq (1077)	559 Uuq (1079)	560 Uuq (1081)	561 Uuq (1083)	562 Uuq (1085)	563 Uuq (1087)	564 Uuq (1089)	565 Uuq (1091)	566 Uuq (1093)	567 Uuq (1095)	568 Uuq (1097)	569 Uuq (1099)	570 Uuq (1101)	571 Uuq (1103)	572 Uuq (1105)	573 Uuq (1107)	574 Uuq (1109)	575 Uuq (1111)	576 Uuq (1113)	577 Uuq (1115)	578 Uuq (1117)	579 Uuq (1119)	580 Uuq (1121)	581 Uuq (1123)	582 Uuq (1125)	583 Uuq (1127)	584 Uuq (1129)	585 Uuq (1131)	586 Uuq (1133)	587 Uuq (1135)	588 Uuq (

authorized database like eChemPortal [2]. I extract the dataset accessed from Wikipedia and many other applications [3]. The original dataset has more than 30 different properties for each element and most of them might be never used by general users. Realizing this fact, I only remain about 10 most common used properties such as melting point, density, and heat of fusion. PerTabVIS visually encodes these properties according to different purposes. For example, the color is used to distinguish different family and the lightness serves for the single property comparison. More details will be illustrated in Section 3.

Many previous applications have focused on the fundamental functions and visualized the periodic table by dyeing table cell with different color and comparing the single property of elements, while there is no such work handling multi-properties comparison and giving users freedom to see the elements distribution according to their interests. In contrast to previous system, PerTabVIS not only remains all of those fundamental functions mentioned above, but also extend the visualized periodic table by providing multi-properties comparison and showing elements distribution according to user interest. The extended contents are very useful. By comparing multi-properties, user can judge whether there is any correlation between different properties. By allowing users to select properties according to their interest, they might discover some features of the corresponding elements distribution. Furthermore, the design of PerTabVIS is also guided by analyzing preference of two target users. The students coming into touch with chemistry in senior school might be interested in seeing elements properties and appearance. But other group, majoring in Chemistry, focuses more on studying the relationship between different properties. That is to say, they involve some comparisons.

I begin by viewing some related work on visualizing periodic table. Next, I present the solution and implementation of PerTabVIS. I then show some screenshots combined with scenarios of use. The results, evaluation, and future work will be discussed in last several sections.

2 RELATED WORK

For an overview on the basic knowledge of the periodic table, I refer the reader to the introduction of Periodic Table on Wikipedia, as this related work section focuses on visualizing the periodic table but not the usage of periodic table.

Visualizing periodic table has been a much concerned topic since it assists so much on chemical research. In this field, early strategy for searching and showing the elements in the periodic table have been introduced by Christopher *et al.* [4]. Most recent researches about the periodic table focus on the web applications. Some of them are like a collecting box of information such as the periodic table in Figure 2 [5]. They collect related information of each element with little derived data. Some of others have a visualized appearance. They dye the table cell with different colors. This is useful to reveal the elements distribution according to period, family, and element type. The elements in each certain group such as transition metal family are dyed with the same color and used different color to differ from others. Denial's work [6] in Figure 3 is a good example. Knoxville and Tennessee create a stronger web application [7] and make some improvements compared with others. They provide single property comparison (as shown in Figure 4), which means to show elements distribution under different cases, such as boiling point and density. The similar work has also been done by Royal Society of Chemistry [8] (as shown in Figure 5).

However, there is no previous work owning the ability to compare multi-properties and giving user freedom to see the elements distribution according to user's interest and selection. To

address these shortcomings and issues, this paper introduces a new visualized tool which contains the functions both in previous work and in those extended contents.

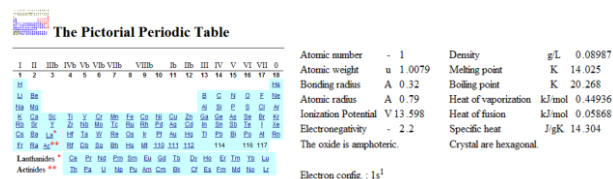


Figure 2. Left: a periodic table like a collecting box. Right: each element directs to a URL containing detailed information

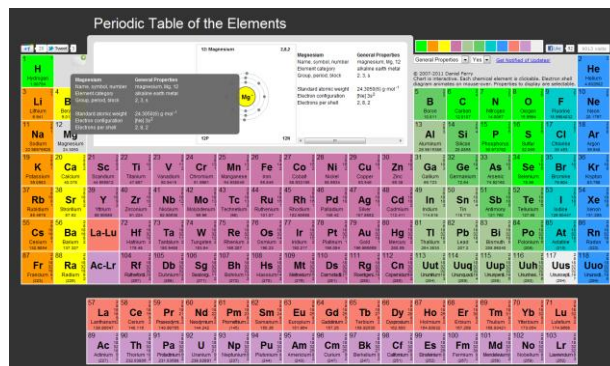


Figure 3. Daniel's Periodic Table

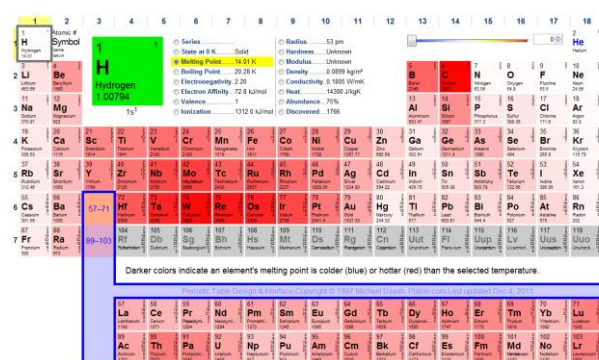


Figure 4. Knoxville and Tennessee's periodic table to compare single property

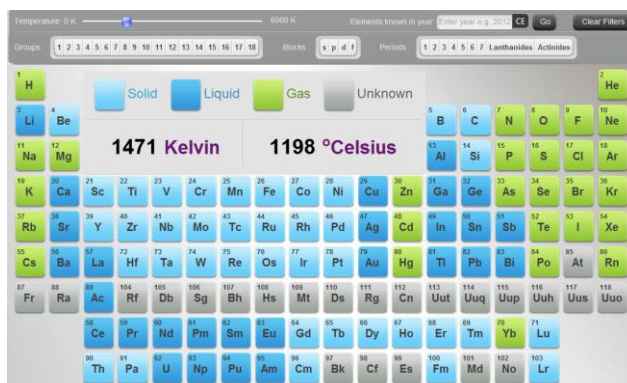


Figure 5. Periodic Table developed by Royal Society of Chemistry

3 DESCRIPTION OF SOLUTION

3.1 Visual Encoding Methods

PerTabVIS mainly uses four types of visual encoding methods, named color, lightness, line, and opacity.

3.1.1 Color

Color is used to encode family (as shown in Figure 6). The elements in the same family have the similar properties. In PerTabVIS, I use 12 different colors to represent 12 different families, respectively.

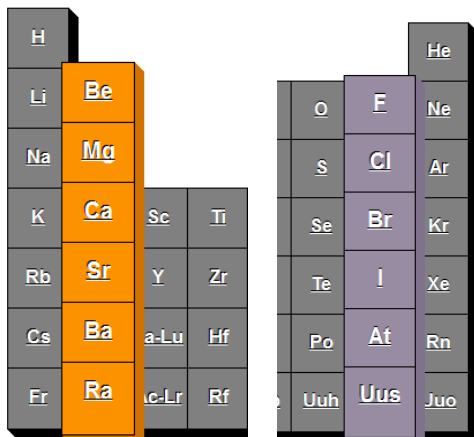


Figure 6. Different color used to differ from families

3.1.2 Lightness

When user asks to compare single property and see the element distribution with the corresponding property, the elements having such property will be encoded with the same color but in different lightness from darker to lighter with value from smaller to larger. For example, when user asks for a comparison of boiling point, the elements will be encoded with orange color (as shown in Figure 7). The dark orange means relatively low boiling point, whereas the light one means relatively high boiling point. Those elements not encoded by any color and lightness means that there is no boiling point for them. So they remain the same in the periodic table.

The gradient of lightness is decided by numerical distribution of corresponding property. The lightness of each element is derived from following equation:

$$lightness_i = \frac{propertyValue_i - \min(propertyValue)}{\max(propertyValue) - \min(propertyValue)} \times 240 \times 0.8 + 36 \quad (1)$$

This equation first maps the numerical value for a property to the lightness range from 0 to 240. Next, to avoid lightness to be too dark as black or too light as white, I clamp the lightness value by linearly transforming it to a somewhat narrower range from 36 to 228.

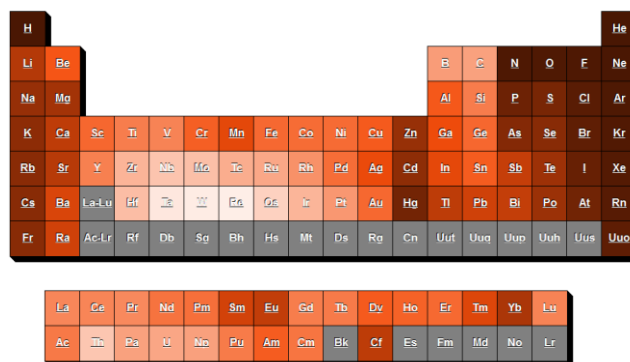


Figure 7. Lightness visual encoding used for boiling point comparison

3.1.3 Line

Line encoding is for parallel coordinate which serves for multi-properties comparison (as shown in Figure 8). Parallel coordinate is very helpful when handling high-dimensional data. The main advantage of parallel coordinate visualization is that it provides an overview and visual insight into correlations of variables which can be easily spotted by lines connecting each axis. PerTabVIS regards multi-properties as high-dimensional data and gives user freedom to filter and highlight interesting region.

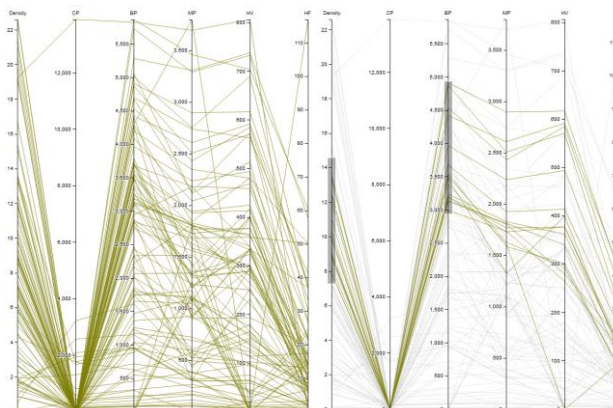


Figure 8. Lines used for parallel coordinate

3.1.4 Opacity

To explore elements distribution according to user selection, I use opacity to differ from those selected and those filtered out (as shown in Figure 9). The opaque elements in the table means what user selects and interests in. By contrast, those transparent elements are filtered out by user. PerTabVIS takes advantages of opacity to clearly reveal elements distribution according to user interest.

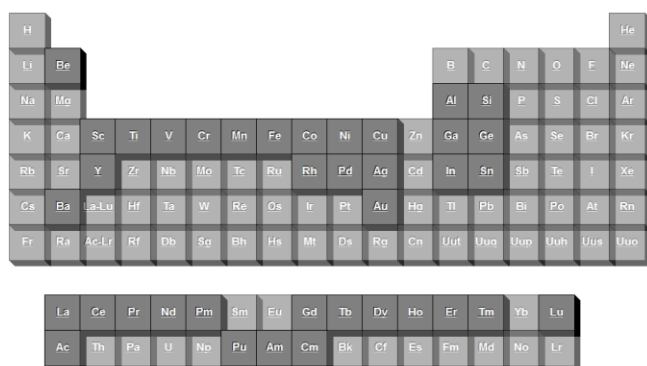


Figure 9. Opacity visual encoding. Opaque ones represent selected elements. Transparent ones are those filtered out

3.2 Panels

There are five panels in PerTabVIS which are main panel, detailed information panel, family panel, single property comparison panel, and multi-properties comparison panel, respectively (as shown in Figure 10).

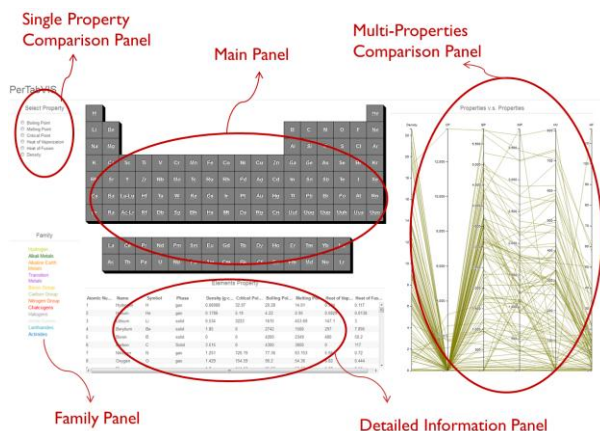


Figure 10. PerTabVIS interface with five panels

3.2.1 Main Panel

The main panel is the periodic table which can also be interactive with other panels. The basic function of this panel is to show the basic information of periodic table, such as element property and appearance. The element will pop out when cursor crosses over it. And the related property information such as density and melting point will be shown beside the cursor. At the same time, the appearance of this element will also be available at the upper of the main panel (as shown in Figure 11). Each row indicates one period. Elements in the same family are encoded by the same color. Besides, the main panel also interactively responds with other panels, which will be explained in later introduction. In short, the main panel is mainly used to display kinds of information such as property, distribution, and comparison result. And when no control happens, it just seems like a traditional periodic table.

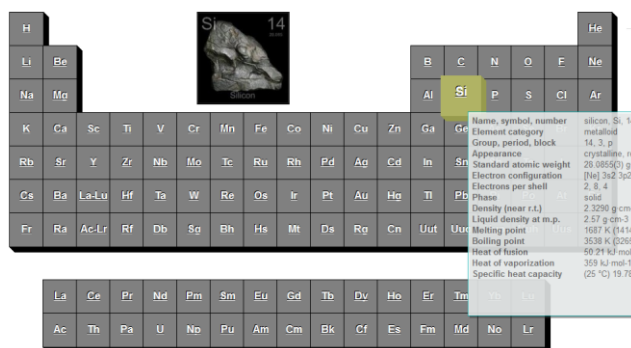


Figure 11. Mouse moving over Si element

3.2.2 Detailed Information Panel

Detailed information panel at the bottom of the webpage is a text grid, which shows all the related information of each element in the order of atomic number increment. When user highlights some properties according to his interest, this panel will be redrawn to remain only the highlighted elements.

3.2.3 Family Panel

Family panel consists of text name of 12 families with different colors. This panel allows user to see elements by group. When cursor moves on a family, the corresponding elements in the same family will all be popped out in the main panel with the same color as that on family text name.

3.2.4 Single Property Comparison Panel

Controls on this upper-left panel aid the user to select single property such as boiling point, melting point, and heat of fusion. A periodic table is represented as the lightness distribution, wherein the darker lightness means smaller value of selected property and elements lacking of such property are invariant.

3.2.5 Multi-properties Comparison Panel

The rightmost panel uses parallel coordinate as a representation of high-dimensional multi-properties. Each numerical property is represented in terms of each vertical axis. The range is evenly divided with the smallest value at the bottom. User can drag each axis to left and right to make it easier to compare (as shown in Figure 12). By brushing the interesting regions (as shown in Figure 13), the highlighted elements will be interactively shown in both main panel and detailed information panel (as shown in Figure 14).


```

<element>
  <number>2</number>
  <symbol>He</symbol>
  <name>Helium</name>
  <property><label>Phase</label><value>gas</value></property>
  <property><label>Density</label><value>(0 °C, 101.325 kPa) 0.1786 g/L</value></property>
  <property><label>Melting point</label><value>(at 2.5 MPa) 0.95 K (-272.20 °C, -457.96 °F)</value></property>
  <property><label>Boiling point</label><value>4.22 K (-268.99 °C, -452.07 °F)</value></property>
  <property><label>Critical point</label><value>5.19 K, 0.227 MPa</value></property>
  <property><label>Heat of fusion</label><value>0.0138 kJ·mol-1</value></property>
  <property><label>Heat of vaporization</label><value>0.0829 kJ·mol-1</value></property>
  <property><label>Specific heat capacity</label><value>(25 °C) 20.786 J·mol-1·K-1</value></property>
</element>

```

Figure 15. Extract dataset and convert it into XML format

5 SCENARIOS OF USE

Several scenarios of use for PerTabVIS are encompassed in the following subsections. More guidelines about how to use this tool can be found in the video demo.

5.1 Viewing Single Element Property

Both the main panel and detailed information panel provide information of each element. A user begins by moving the cursor to the target element. Perhaps the user is interested in the element *Si* but have no idea about it, even for the full name and atomic number. Move the mouse and stop at *Si* position (as shown in Figure 11). The *Si* element will pop out and related information about *Si* will be displayed in the text window besides the cursor (as shown in Figure 16). Then, the user knows *Si* represents Silicon and the atomic number is 14th. And other useful information such as density, phase, and boiling point will be emerged together. Moreover, the corresponding image which indicates what *Si* looks like will be drawn on the top of current main panel (as shown in Figure 11). Then, the user wants to write it down to the note book in case of forgetting it later. So he moves the mouse to the notepad and the text window of element information disappears thereupon. Don't worry about it. PerTabVIS also has a text grid in the detailed information panel which records all the properties for each element. The user then comes back to the tool and finds the 14th element in the text grid (as shown in Figure 17). At this time, he can contentedly write all the knowledge points down.

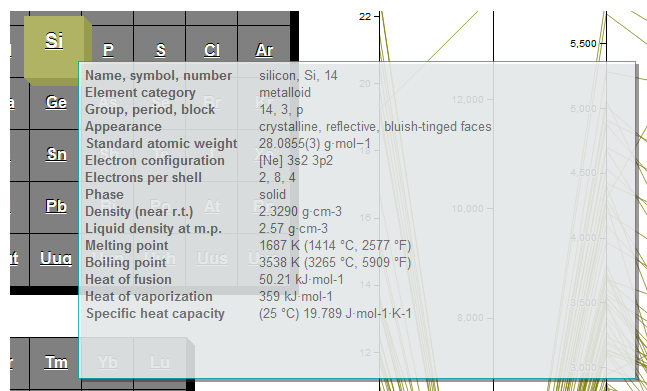


Figure 16. Text window includes all the information

Atomic Nu...	Name	Symbol	Phase	Density (g·c...	Critical Poi...	Boiling Poi...	Melting Poi...	Heat of Vap...	Heat of Fus.
13	Aluminum	Al	solid	2.7	0	2792	933.47	294	10.71
14	Silicon	Si	solid	2.329	0	3538	1687	359	50.21
15	Phosphorus	P	solid	2.69	0	550	317.3	12.4	0.66
16	Sulfur	S	solid	1.92	1314	717.8	388.36	45	1.727
17	Chlorine	Cl	gas	3.2	416.9	239.11	171.6	20.41	6.406
18	Argon	Ar	gas	1.784	150.87	87.3	83.8	6.43	1.18
19	Potassium	K	solid	0.89	0	1032	336.53	0	0
20	Calcium	Ca	solid	1.55	0	1757	1115	154.7	8.54

Figure 17. Text grid also shows all the information of Si

5.2 Viewing Elements In A Family

Using the family panel, the user can see the corresponding elements belonging to the selected family at one time. A user might be curious about which elements are in the category of noble gases. Move the mouse to family panel and stop the cursor at grey text named *Noble Gases* (as shown in Figure 18 left). In the main panel, the elements belonging to this family will pop out with same grey background color (as shown in Figure 18 right).

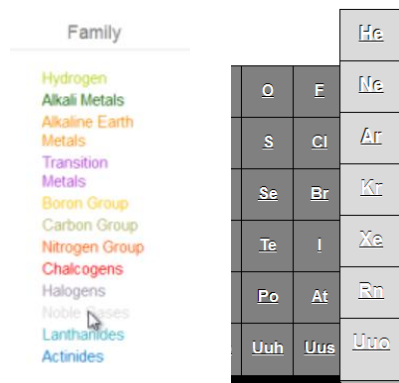


Figure 18. The elements belonging to Noble Gases family popped out with the same grey background color

5.3 Single Property Comparison

Let us imagine that a user is solely interested in the elements distribution with melting point. Click on the radio button *Melting Point* in the single property comparison panel and the periodic table in the main panel will be encoded with different level of lightness (as shown in Figure 19). Hydrogen *H* is encoded by a very dark red which means it has a relatively quite low melting point. Tungsten *W* with a very light orange indicates its such high melting point. Actually, tungsten is the raw material of lamp filament. Thus, it is also reasonable that tungsten has a relatively high melting point.

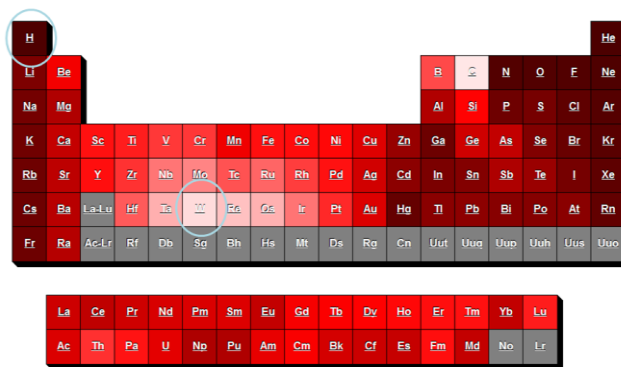


Figure 19. Single Property Comparison of melting point

5.4 Multi-properties Comparison

After comparing the single property, perhaps the user wants to explore deeper relationships between different properties, such as correlation. For instance, the user might have a previously formed hypothesis that the melting point and heat of fusion are the same concept or correlated with each other since the definition of these two concepts seems somewhat similar. So he drags the axis of

melting point to make these two properties closed (as shown in Figure 20 left). As a result, the fact overturns his wrong assumption because the crossing lines connecting two axes indicate no correlation (as shown in Figure 20 right).

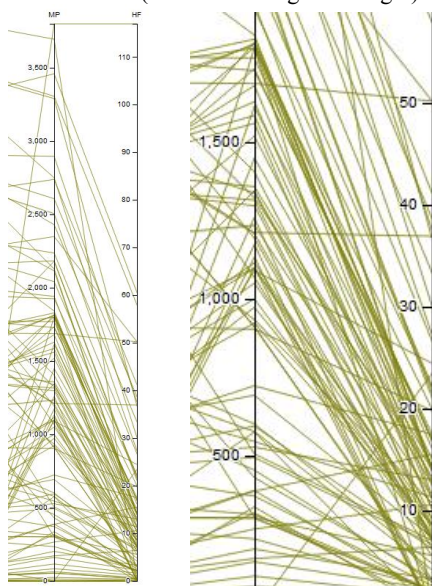


Figure 20. Left: Move the MP axis close to HF axis. Right: No correlation between two properties

5.5 Explore Elements Distribution Under Certain Situation

There is a question of how about the elements distribution with those having relatively low density but owning high boiling point? The user then brushes the region on the density axis for the relatively low value and also selects the upper half of boiling point axis. The highlighted lines now are the intersection for elements with low density and high boiling point (as shown in Figure 21). As a result, the corresponding elements distribution in the main panel reveals that elements having such property are almost the transition metals (as shown in Figure 22).

Another scenario is to explore elements distribution with both low boiling point and low melting point (as shown in Figure 23). In the same process, the user filters the elements and discovers that no transition metals have such property except mercury *Hg* (as shown in Figure 24). He then searches the Wikipedia to find the answer. Mercury [11] is the only metal that is liquid at standard conditions for temperature and pressure because of very weak Van der Waals' force¹.

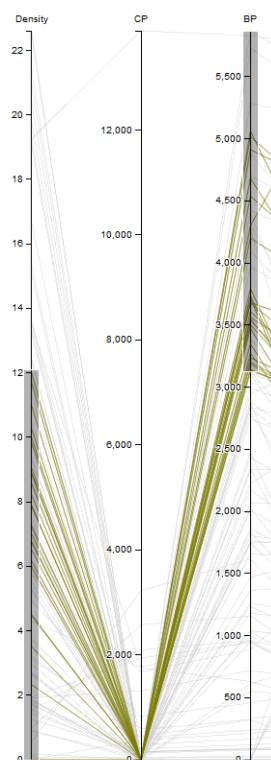


Figure 21. Brush the regions on two interesting regions

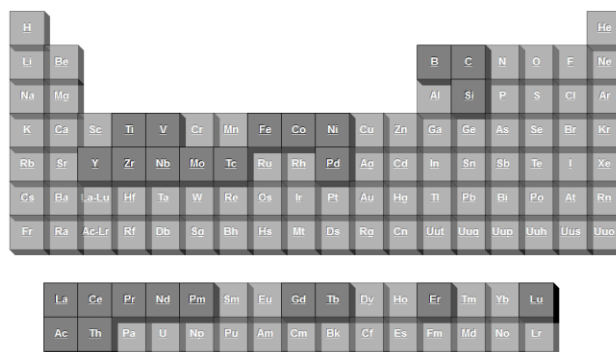


Figure 22. Elements having such property are almost the transition metals

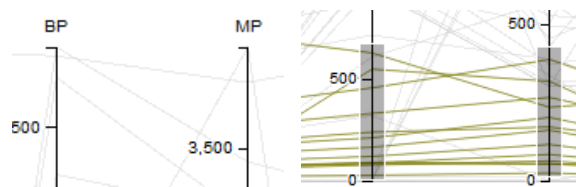


Figure 23. Filter elements having both low boiling point and low melting point

¹ Van der Waals' force [12] include attractions between atoms, molecules, and surfaces, as well as other intermolecular forces

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La-Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac-Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Uuq	Uup	Uuh	Uus	Uuo
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			

Figure 24. Hg is the only metal having such a low boiling and melting point

6 RESULTS

The section above has already shown what PerTabVIS can do and how it can be used. So I just want to give a brief conclusion in this section.

To summarize, PerTabVIS provides the basic function for the chemical tyro such as showing the element properties and displaying elements belonging to the same family. For the upper level user majoring in Chemistry, PerTabVIS supports two types of comparison, named single property comparison and multi-properties comparison respectively. And PerTabVIS even allows user to explore the elements distribution according to user selection and interest.

7 DISCUSSION AND FUTURE WORK

7.1 Strengths and Weaknesses

7.1.1 Strengths

PerTabVIS presents a new method to visualize the periodic table. By remaining the basic function in previous work and extending comparison for upper level user, PerTabVIS is qualified to be an effective and useful visualized tool when learning and exploring chemistry. The strengths of PerTabVIS are embodied in following parts.

First, PerTabVIS supports both single property comparison and multi-properties comparison. This feature is very useful to explore the elements relationship. And the parallel coordinate served for multi-properties comparison is also very helpful with regard of its effective expression of relationship among high-dimensional data.

Another contribution of PerTabVIS is to provide users freedom to select what they are interested in and therefore create a possibility to discover some valuable feature from corresponding elements distribution.

One more strength of PerTabVIS is in its accessibility to all kinds of users. As a web application, the only requirement to users is that they must have a computer at hand and also internet accessible. Even for the color blindness, the comparison of property is also available, since PerTabVIS encodes the single property comparison and multi-properties comparison with lightness and opacity respectively. These two kinds of visual encoding methods are known as color-blind free (as shown in Figure 25 and Figure 26).

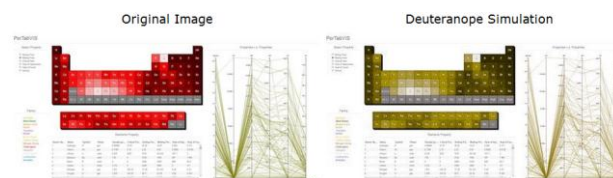


Figure 25. No obstruction for color blindness to distinguish different lightness

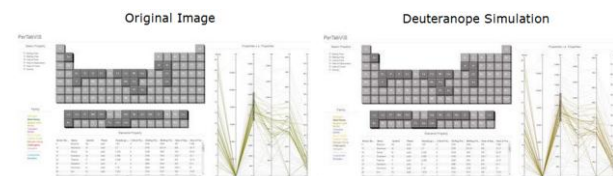


Figure 26. No obstruction for color blindness to differ opacity

Besides, the good interactivity is another obvious advantage. Interactivity reflects into two parts: users are interactive with the interface and panels are also interactive with each other. The interactivity therefore brings perfect user experience and also effectively expresses more meaningful information at the same time.

7.1.2 Weaknesses

However, I think this tool could see a number of improvements. First, although PerTabVIS benefits from parallel coordinate served for multi-properties comparison, it is also up against the clustering issue. The cluster might impede the accuracy of evaluating multi-properties relationship. Users are even subject to coarsely select their interested region.

Second, PerTabVIS fails to support bidirectional linking between the main panel and multi-properties comparison panel. Specifically, user cannot select the interesting elements from the periodic table and explore their properties distribution in parallel coordinate used for multi-properties comparison. For example, it is the common sense that elements in the same family have somewhat similar properties. If users want to see what actually these similarities are, they involve this directional linking from main panel to multi-properties comparison panel. By doing this, PerTabVIS will also be more robust and functional. Unfortunately, due to the time limitation, current PerTabVIS doesn't support this mechanism. So I prefer to set this aside for the future work.

Another shortcoming is also given arise to the limited time. By now, PerTabVIS has only supported comparison for six properties. However, I believe there must be much more valuable outcomes derived by comparing more various properties. It is not only involved into extending the size of dataset, but also designing new visual encoding methods.

7.2 Reproducibility

This project is reproducible for following reasons.

7.2.1 Code Reproducibility

PerTabVIS utilizes third-party open-source library, such as d3.js and SlickGrid. In addition, since this tool is a client-side web-based application, all the source codes can be even obtained from any client browser.

7.2.2 Data Reproducibility

The dataset used in PerTabVIS is extracted from web resource. And I also publish dataset I used. So it is available for anyone to get it and reuse it.

7.2.3 Reference Reproducibility

All the references at the end of the paper can be accessed through Internet for free.

7.3 Lessons Learned

7.3.1 Project Scope

How to draw up project scope is one crucial lesson I have learned. The difficulty of real implementation is far beyond what I have thought in my initial blue-print. In my project proposal, I imagined lots of functions. Some of them are proved to be useful and occurs in the final project. But some others are really nonsense because I had never thought who will be my target user and how to implement them. I also failed to analyze the previous work. I have a general lack of understanding what previous work has already done and what I can improve. Even for the dataset, I had envisioned there will be lots of available source on the internet not having to be manually probed and reorganized since periodic table is widely used. Actually speaking, I have suffered delays and setbacks caused by aforementioned problems and oversights. As a result, a rational and logical project scope cannot be more significant. It is worth thinking twice before drafting proposal.

7.3.2 Communication

Communication with instructor and other mates is very helpful. They give me many constructive suggestions. But when I realized this point, it is a little bit late. I start to ask others evaluation even after update presentation. I waste lots of time on some of my initially wrong assumption. It leads to my much more work in these last three final weeks. Anyway, I have learned this lesson.

7.3.3 Just Do It

Thinking twice before bring into action is encouraged and needed. But excessive hesitation should be denied. When deciding which toolkits should be used to implement PerTabVIS, I went through a hard time. The d3.js is such an up-to-date tool that I am fearful of few help document of it. Thus, I even produced the intention to give up it and use other toolkits. On the other hand, I am also attracted by its power to make implementation of parallel coordinate very easy. I then hover over whether to use it or not for several days. Although finally I still decide to use d3.js, to make this decision wastes me couple of days. From this experience, I have learned that just do it as long as you think it is powerful enough. Learning the novel technique seems not too bad.

7.4 Future Work

PerTabVIS is just a course project now. So it is far away from perfectness. There is a number of improvements worth to do according to the weaknesses I discussed above. First, I plan to make use of “focus + context” technique to overcome clustering issue caused by parallel coordinate. This technique is known as effectively addressing the cluster problem in terms of zooming in and extending the focused region but zooming out and compressing other contexts. Another future work is to add bidirectional linking between the main panel and multi-properties comparison panel. The significance for doing it has already been illustrated. Since extending the dataset will definitely reveal more relationship, it is also on my to-do list.

REFERENCES

- [1] Dmitri Mendeleev
http://en.wikipedia.org/wiki/Dmitri_Mendeleev
- [2] eChemPortal
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- [3] Dataset from other applications
<http://www.excelhero.com/periodic-table/>
- [4] Christopher Ahlberg , Christopher Williamson , Ben Shneiderman, Dynamic queries for information exploration: an implementation and evaluation, *Proceedings of the SIGCHI conference on Human factors in computing systems*, p.619-626, May 03-07, 1992, Monterey, California, United States
- [5] The pictorial periodic table
<http://dwb.unl.edu/Teacher/NSF/C04/C04Links/chemlab.pc.maricopa.edu/periodic/periodic.html>
- [6] Daniel Ferry's Periodic Table of Elements
<http://www.excelhero.com/periodic-table/>
- [7] Knoxville and Tennessee's Ptable
<http://www.ptable.com/?lang=en>
- [8] Visual Element Periodic Table developed by Royal Society of Chemistry
<http://www.rsc.org/periodic-table/>
- [9] d3.js
<http://mbostock.github.com/d3/>
- [10] SlickGrid
<https://github.com/mleibman/SlickGrid/wiki>
- [11] Mercury
[http://en.wikipedia.org/wiki/Mercury_\(element\)](http://en.wikipedia.org/wiki/Mercury_(element))
- [12] Van der Waals' force
http://en.wikipedia.org/wiki/Van_der_Waals_force