Interactions and bonds between alkali metals and noble gases at high temperature
Computational Chemistry

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The motivation for this study came from a question that I could not easily find an answer to. Will an ionized noble gas bond with an alkali metal at high temperatures similar to that of molecules like $NaCl$? The results were different than expected, but not surprising.

First lets look at how the energy compares to the bond length of each pair.

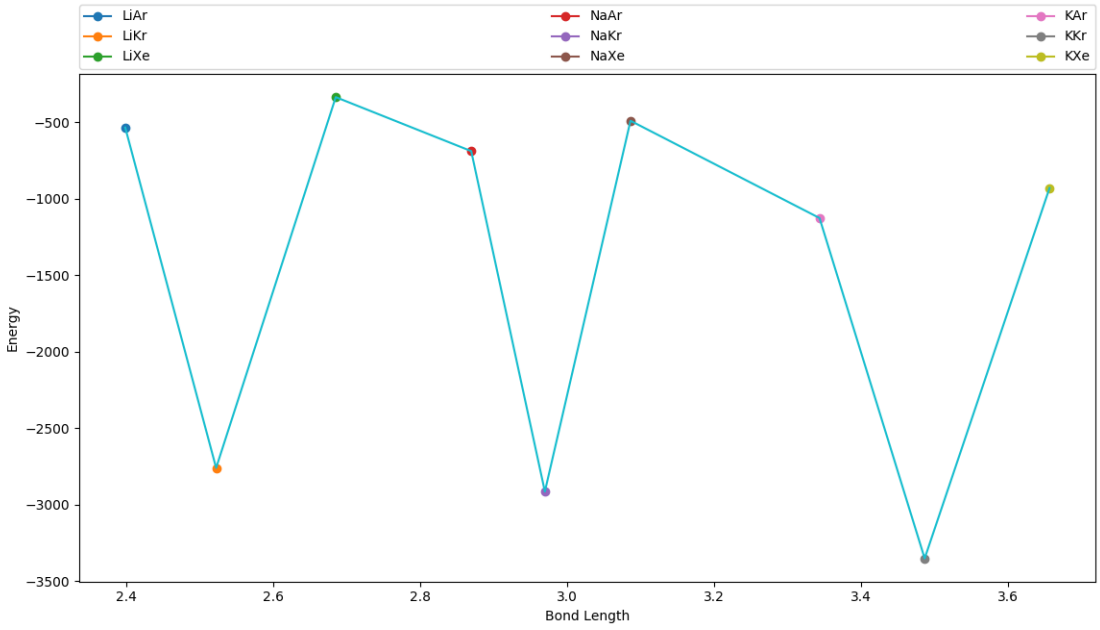


Figure 1: Bond Length vs Energy

It can be seen from the plot above that the pairs with a krypton atom have lower energy that those with argon or xenon. This is because the larger the atoms the lower the energy should become due to the increase in protons of the system. However this

is not the case with xenon. I believe this is because for xenon a pseudopotential had to be used. A pseudopotential is a potential this approximates the contributions from inner core electrons.

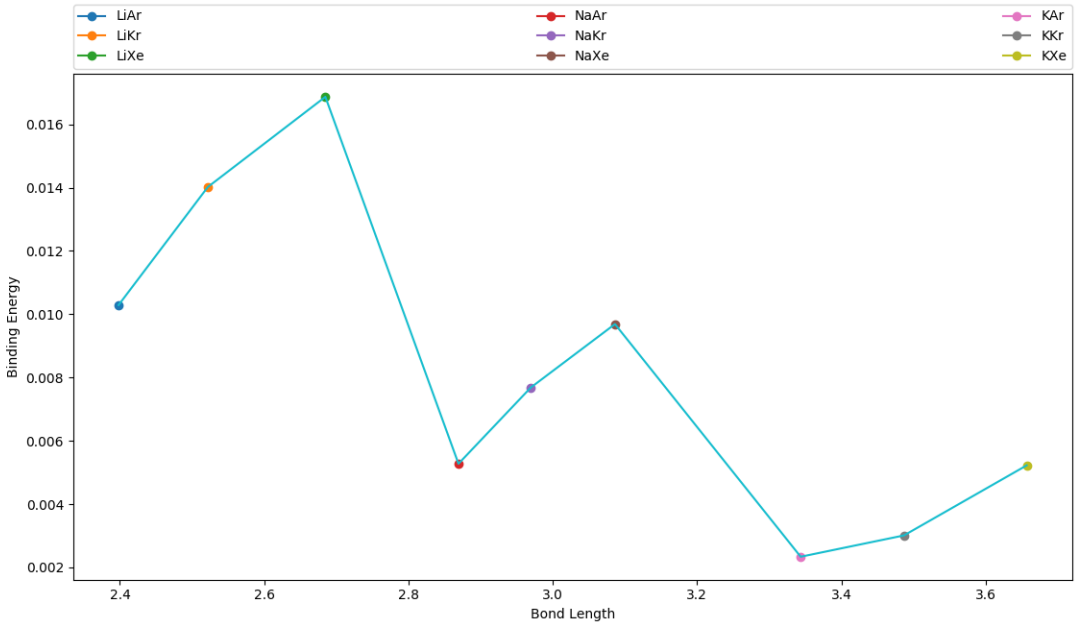


Figure 2: Bond Length vs Binding Energy

Since there is not much data on these molecules there is not an experimental bond length for most of them. To validate my results I ran three different bond lengths; one angstrom, four angstroms, and 7 angstroms. Then used the one closest to the optimized length to find the energy. These bond lengths were then compared to the binding energy in the plot above. As expected, as the bond length increases the binding energy decreases.

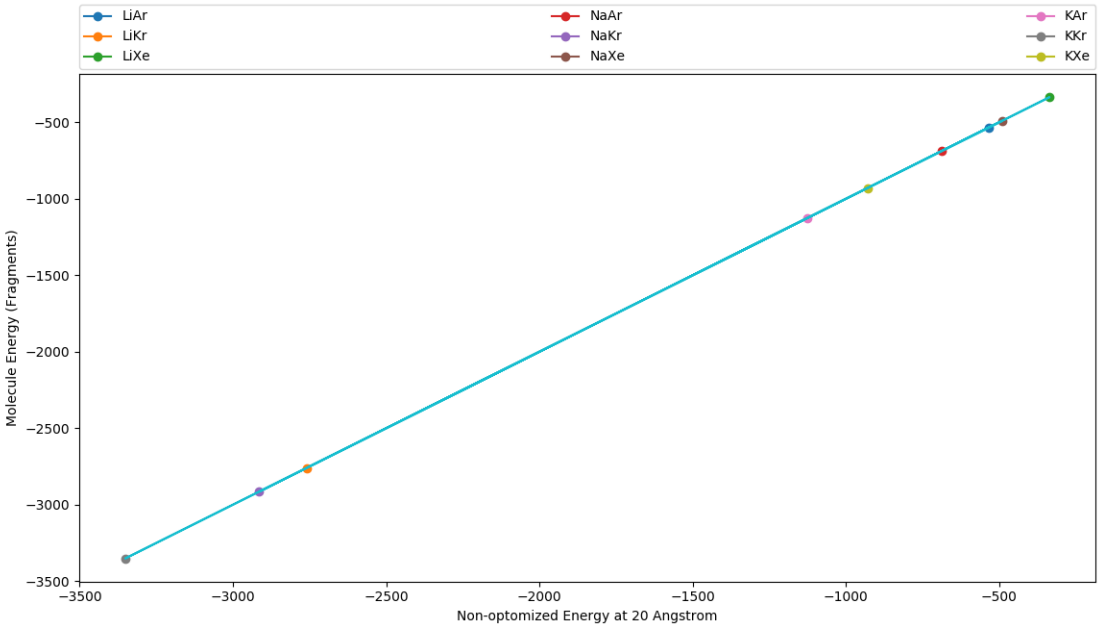
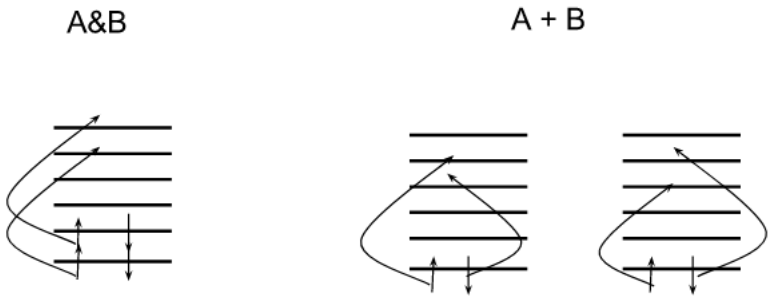


Figure 3: Size Consistency

The above plot represents the size consistency, this was something used to help validate my results. The y-axis is the energy of each atom added together for each pair, and the x-axis is the energy that was found when the atoms are twenty angstroms apart. What is important here is that the axis have the same scale, if x equals y for every point then we can trust our results. This also demonstrates that the methodology used is size consistent. Being size consistent means that the methodology allows for for more than just singly and doubly excited states. If the methodology was not then this plot would not be a one to one plot. Below is a picture to help explain the difference in allowed excited states.



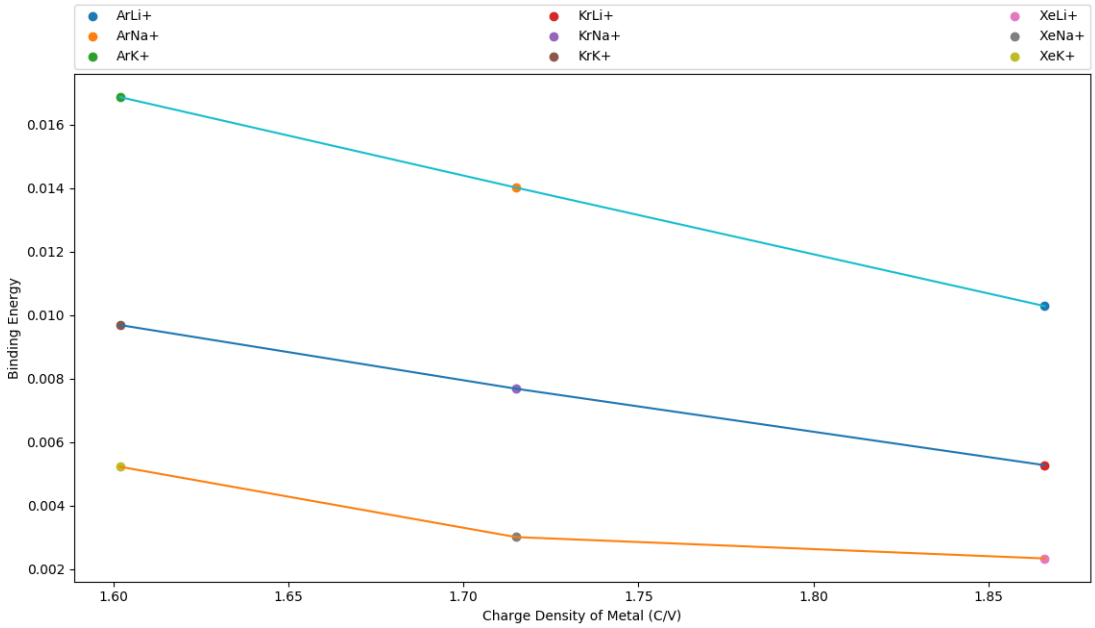


Figure 4: Charge Density vs Binding Energy

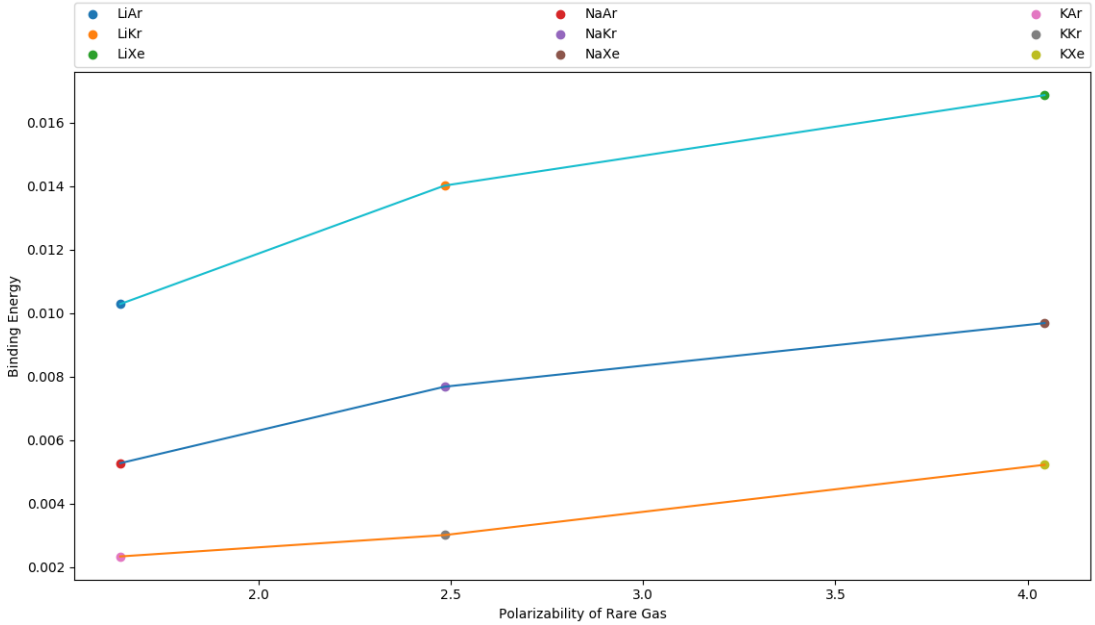


Figure 5: Polarizability vs Binding Energy

Now lets look at some trends among the atoms involved and how they affect the results. First is the charge density of the alkali metals used. It is important to note that

the charge does not change as the element does. Each atom has the same number of electrons and protons, increasing proportionally as you move down the periodic table. Removing one electron from each will leave a positive charge equal to the charge of one proton. All that will change then is the volume of the atom. Using the volume of a sphere and the radius of each atom I was able to calculate the charge density for each metal. As the charge density increase the binding energy decreases. This also implies that if the volume of the alkali metal increases then the binding energy will also increase. The next property looked at was the polarizability of the rare gases. These values were found from experimental results and then compared to the binding energy. As the polarizability increases so does the binding energy, this is as expected. It is also important to note that the as you move down the periodic table the polarizability increases. This is because as the atoms become larger, the electrons mover further and further away from the core, allowing them to be influenced by external fields easier.

To sum up the project, the results were not surprising. All of the alkali metals carry the charge in the molecules, even if the rare gas was ionized and then introduced to the metal. Once fully relaxed and at the lowest energy the charge will have moved to the alkali metal.