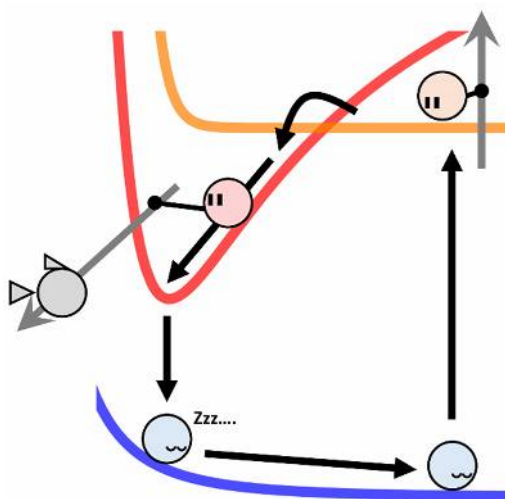


Unfamiliar terrain in the microscopic world

Yosuke Asami (Department of Chemistry)



I am a graduate student in the department of chemistry. I am interested in dynamics of molecules, which are extremely small (about 0.0000000001 m elemental components of materials), and I observe them in vacuum. In this essay, I will tell you what is interesting in my study.

As you know, rivers run from mountains to the sea. When you drop a basket of apples on a slope, the apples roll down. These facts show that objects tend to go from high to low. As you know, the rule is valid in the world you can see, but is it also valid in the molecular world? The answer is partially yes, and partially no.

Like human-scale objects, molecules also proceed from "high" to "low". However, for molecules, gravity does not determine where is "high" and where is "low" because they are too light (about 0.00000000000000000001 g) to feel little gravity. Instead, electric force provide "terrain" for molecules to push them to a lower place. What is important is that those forces often form unique "terrain", which causes strange movement of molecules. Such dynamics are not only interesting but also important for some practical applications.

The harpooning effect is a good example of dynamics due to the unique "terrain" [1]. The harpooning effect appears when two neutral molecules or atoms, one of which (named as Prey) prefers to take an additional electron and the other (named as Hunter) prefers to throw away one electron, approach each other. At first, they feel little force because they have no charges. In other words, Prey and Hunter are on the flat "terrain" at that time. When they reach a certain distance, one electron transfers from Hunter to Prey suddenly, Hunter and Prey come to have positive and negative charge, respectively, and they begin to attract each other by electric force. In this phenomenon, Hunter and Prey jump from the "plain" to the "slope" immediately. Finally, they get close and combine to be Prey-Hunter (this is as if Hunter catches Prey by stabbing it with an electron as a harpoon, and that is why this process is called as harpooning effect). That is how the harpooning effect proceeds: Hunter and Prey switch the "terrains" at the beginning of the reaction. Thanks to the harpooning effect, reactions of alkali metal atoms (corresponding to Hunter) and halogen molecules (corresponding to Prey) occur over a long distance.

Unique dynamics of molecules is not merely surprising but also potential for practical application. That is why I am interested in the field. Let me take an example as the harpooning effect again. Harpooning effect is applied for designing lasers [1]. Laser (Light Amplification by Stimulated Emission of Radiation) is a device to emit light with useful features such as high intensity and high directivity. Operating lasers requires population inversion in the light source: the number of molecules with high energy has to be larger than that of molecules with low energy. Achieving population inversion is challenging, but the harpooning effect can realize it.

The laser gains light from the reaction of two kinds of gas molecules (named Sleeper and Prey). The reaction involves jumping among three "terrains". First, Sleeper and Prey move on the "low energy terrain", which rapidly rises when Sleeper and Prey get too close. Sleeper is

often stimulated, or “waken up”, to be Hunter, and the harpooning effect, involving the two "high energy terrains", starts. The resulting Prey-Hunter, , throw away their excess energy as light to be Prey-Sleeper. Because it is on the first "low energy terrain", Sleeper immediately goes down the "slope" to go apart from Prey, and finally, Sleeper and Prey return to the initial state. In the whole reaction, the species related to the light emission are Prey-Hunter and Prey-Sleeper, the former is the molecule with high energy, and the latter is that with low energy. Prey-Hunter is abundant thanks to the harpooning effect, whereas Prey-Sleeper is scarce due to the "steep slope". As such, the excimer laser achieves population inversion. As this example shows, knowledge of the dynamics of molecules provided by the "terrain" is useful for our society.

The shape of the "terrain" is essential for understanding the behaviors of the molecules. Then, how do we acquire the information about the "terrain"? Many experimental ways have been developed, and I have chosen the observation of molecules in a vacuum. Molecules introduced into vacuums feel no force from other molecules, so you can investigate the "terrain" formed on the molecules themselves and their movement on the "terrain" by observing such isolated molecules. Of course, it is possible to observe the movement of molecules in a solvent (e.g. water), but such molecules interact with a lot of neighboring molecules, and analyzing the behavior of the molecules is difficult. Therefore, we can access fundamental information on the movement of molecules with vacuum experiments.

Although molecular dynamics and vacuum experiments are fields of chemistry, they require knowledge and skills in a wide variety of scientific and engineering fields. Knowledge of material science is essential to finding interesting questions to solve with the vacuum experiments. Skills for considering the behavior of materials based on physics let you come up with an idea of what physical phenomena are useful to detect the nature of the target materials. Engineering skills help you to design, build, and modify the apparatus. In this way,

performing vacuum experiments demands combining many kinds of skills. Only learning chemistry is far from sufficient to conduct such experiments. It is essential to learn wide fields, including physics, mathematics, and engineering.

Reference

[1] Levine, R. D. *Molecular Reaction Dynamics*; Cambridge University Press, 2005.

Grammarly is used to correct grammar mistakes.

I would like to thank Prof. Mark Vagins and peer reviewer Mutsumi Shimomura for giving me some fruitful advice to improve this essay.