CASE 34

“ChemPark”
About a Cloud Service for Chemical Computing
～New Approach Case for the Digital Native Generation～

Content

“ChemPark” is provided by HPC Systems that is the niche top company of the field of high-performance computing in Japan

HPC Systems hope that this whitepaper would give an image of the cloud service for chemical computing

About the User

National University Corporation
Shizuoka University

Shizuoka University is one of the leading universities in Japan, established in 1949. The University offers a wide range of disciplines keeping up-to-day with the world education trend. One of the good examples is the department of engineering. While most of the universities provide either physics or chemistry experiment facility for students, Shizuoka University offers both physic and chemical experiments under the same environment. That means the students can learn their interested subjects, which could be associated to a wider discipline area of knowledge in science.

The university's philosophy is “Freedom and Enlightenment for Creation of the Future”. The idea is nurturing students in a free environment without restriction and respecting each student’s individuality for them to develop their own potentials and talents. With that, the department provides a chemical experiment tool to all students regardless their disciplines. So, the students can have the opportunity in chemistry experimental practice, without being bound by or too focused on a single study area.

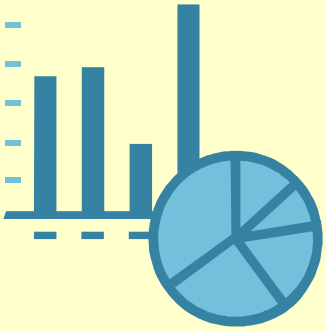
Also, the location (Hamamatsu) of Shizuoka University is the bases of many automobile manufacturing leaders of the world, like Toyota, Honda and Suzuki. Therefore, the Department of Engineering has been always incorporating with the local industry to offer students the most practical educations.

550 students use “ChemPark”

From 2019, The Department of Engineering in Shizuoka University are using “ChemPark” (a cloud service for chemical computing) for their teaching materials in classes. Shizuoka University use it for the chemical experiment in the course that all of the sophomore has to attend. As it is a required subject, about 550 students attends it every year. The course is not only for the students specialize in chemistry, it’s for students who aim for a variety of specialized fields, such as mechanical, electrical and electronic, and mathematical systems engineering.

CHALLENGES

- *Design a lecture with the latest computational science with a limited budget*
- *Introduce computational science without problems in the future*



Check “ChemPark” at

HPC Systems Inc.
https://www.hpc.co.jp/

HPC System is always ready to provide researchers the power to research and the developers the power to develop products.

Why “ChemPark”?

As computational science is spreading in various fields, there are more and more laboratories in the chemical field that not only use experiments but also computational chemistry. Shizuoka University believes that computational chemistry will become more important in the future, so they introduced “ChemPark” from the latter half of 2019.

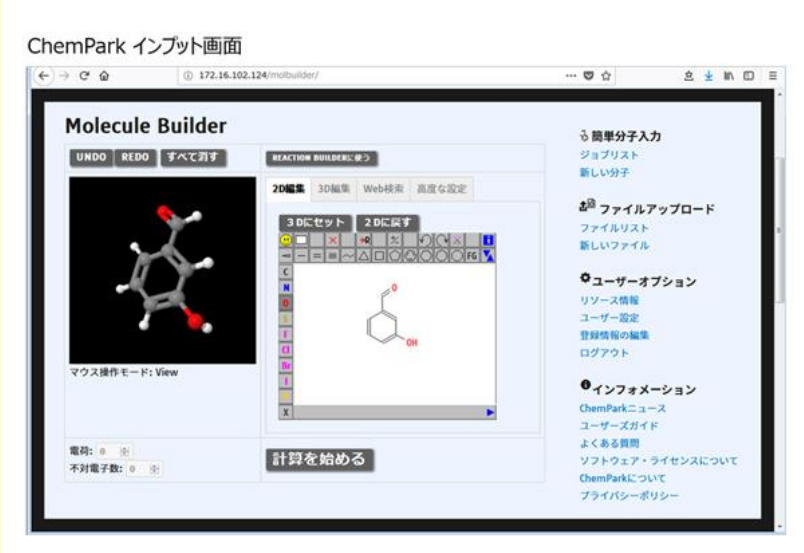
Shizuoka University’s limitation was that it was quite difficult to install the machines and purchase the software license for each student because of the limited budget. Another limitation was about manpower, there wasn’t enough people that can install software in the initial introduction and to maintain it in the future.

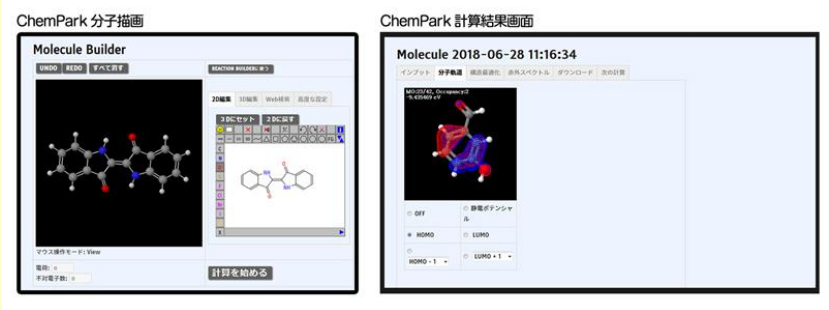
By considering these circumstances, Shizuoka University came to the conclusion that the only way they could use computational chemistry in classes, would be using it through cloud services. So, Shizuoka University started looking for a cloud service and found “ChemPark”.

With “ChemPark”, Shizuoka University only needed to get the machines ready, and it was not necessary to maintain the system regularly, and there was no need to purchase a license for each student.

“ChemPark” was easy to start.

“ChemPark” Input Screen





How students use “ChemPark”

The students in Shizuoka University are mainly computing predetermined molecules with “ChemPark”.

The experiments using “ChemPark” are conducted by the information they have already learned in their first year, so the theme of “ChemPark” is to actually compute and consider with their own knowledge. As students in all departments learn about basic chemical engineering in the first year, students use “ChemPark” for three main things: total energy, orbital energy and molecular orbitals.

Shizuoka University aims those students learn more by using their own knowledge and actually computing and checking what they already know.

Lavatory

Professor Kazumasa Ueda

・Chemistry and Biochemical Engineering Course of Department of Engineering in Graduate School of Integrated Science and Technology

・Professor Kazumasa Ueda’s Laboratory

URL : https://wwp.shizuoka.ac.jp/uedalab/

・Research Field: Development of near-infrared light absorbing materials and development of organic crystals with nano-sized vacancies

Associate Professor Keiko Miyabayashi

・Chemistry and Biochemical Engineering Course of Department of Engineering in Graduate School of Integrated Science and Technology

・Laboratory

URL :https://wwp.shizuoka.ac.jp/miyabayashi-lab

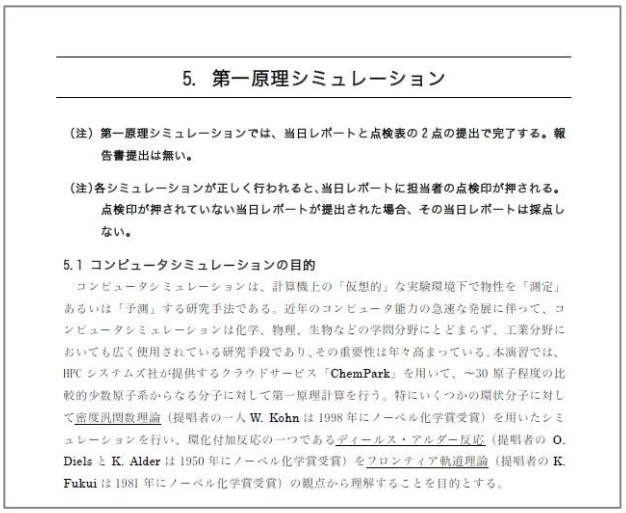
・Research Field: Surface modification of metal nanoparticles and application to electrochemistry

Associate professor Yoshifumi Noguchi

・Chemistry and Biochemical Engineering Course of Department of Engineering in Graduate School of Integrated Science and Technology

・Research Field:Development and Application of the first principle of Green function method

“ChemPark” Textbook



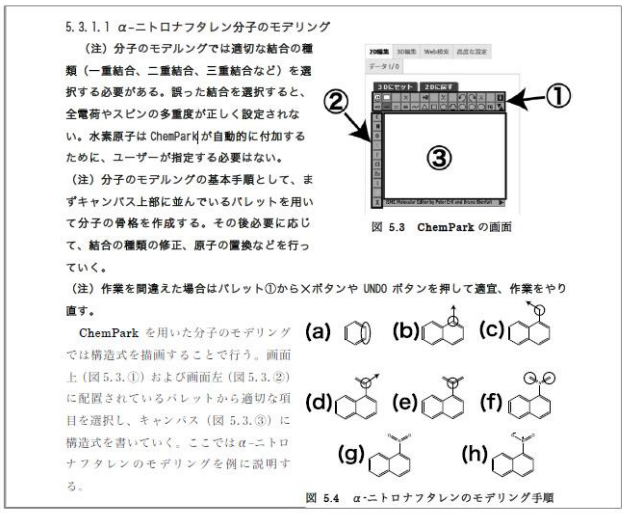
5. 第一原理シミュレーション

（注）第一原理シミュレーションでは、当日レポートと点検表の 2 点の提出で完了する。報告書提出は無い。

（注）各シミュレーションが正しく行われると、当日レポートに担当者の点検印が押される。点検印が押されていない当日レポートが提出された場合、その当日レポートは採点しない。

5.1 コンピュータシミュレーションの目的

コンピュータシミュレーションは、計算機上の「仮想的」な実験環境下で物性を「測定」あるいは「予測」する研究手法である。近年のコンピュータ能力の急速な発展に伴って、コンピュータシミュレーションは化学、物理、生物などの学問分野にとどまらず、工業分野においても広く使用されている研究手段であり、その重要性は年々高まっている。本演習では、HPC システムズ社が提供するクラウドサービス「ChemPark」を用いて、～30 原子程度の比較的少数原子系からなる分子に対して第一原理計算を行う。特にいくつかの環状分子に対して密度汎関数理論（提唱者の一人 W. Kohn は 1998 年にノーベル化学賞受賞）を用いたシミュレーションを行い、環化付加反応の一つであるディールス・アルダー反応（提唱者の O. Diels と K. Alder は 1950 年にノーベル化学賞受賞）をフロンティア軌道理論（提唱者の K. Fukui は 1981 年にノーベル化学賞受賞）の観点から理解することを目的とする。



5.3.1.1 α-ニトロナフタレン分子のモデリング

（注）分子のモデルングでは適切な結合の種類（一重結合、二重結合、三重結合など）を選択する必要がある。誤った結合を選択すると、全電荷やスピンの多重度が正しく設定されない。水素原子は ChemPark が自動的に付加するために、ユーザーが指定する必要はない。

（注）分子のモデルングの基本手順として、まずキャンバス上部に並んでいるパレットを用いて分子の骨格を作成する。その後必要に応じて、結合の種類の修正、原子の置換などを行っていく。

図 5.3 ChemPark の画面

（注）作業を間違えた場合はパレット①から×ボタンや UNDO ボタンを押して適宜、作業をやり直す。

ChemPark を用いた分子のモデリングでは構造式を描画することで行う。画面上（図 5.3.①）および画面左（図 5.3.②）に配置されているパレットから適切な項目を選択し、キャンバス（図 5.3.③）に構造式を書いていく。ここではα-ニトロナフタレンのモデリングを例に説明する。

(a) (b) (c) (d) (e) (f) (g) (h)

図 5.4 α-ニトロナフタレンのモデリング手順

Textbooks are provided for computer use, but “ChemPark” can also be accessed from a smartphone. In fact, students use smartphones to conduct exercises and even uploads assignments from their smartphones.