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Development of Online Quantum Chemistry Experiment Environment Based on Computational Science Platform

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ABSTRACT

This paper introduces an online experiment environment based on a computational science platform that can be used for various purposes ranging from basic education to quantum chemistry and professional quantum chemistry research. The simulation environment was constructed using a simulation workbench and simulation workflow, which are execution environment services of Science App provided by the computational science platform. We developed an environment in which learners can learn independently without an instructor by selecting experiment topics that can be used in various areas of chemistry, and offering the learning materials of the topics in a form of e-learning content that includes theory and simulation exercises. To verify the superiority of the proposed system, it was compared with WebMO, a state-of-the-art web-based quantum chemistry simulation service.

☞ keyword : Computational Science Application, Computational chemistry

1. Introduction

The use of computational chemistry for basic topics such as quantum mechanics or reaction kinetics, which are normally delivered in a unilateral form of knowledge transfer, enables a concrete understanding of various concepts by providing practical calculation experiments. Computational chemistry can directly assist with chemistry education by visualizing how the knowledge learned through textbooks is applied to actual experiments and research. Further, utilizing the cyber infrastructure developed for computational chemistry can lead to a wide variety of convenient academic environments, and can also be used to effectively educate young scientists in the chemistry field. Unlike traditional education that focuses on physical experiments, the nature of the Internet enables easier access to experiments using a PC without being tied to a physical space. In addition, there is an advantage in that once the cyber infrastructure is deployed, the maintenance cost is much cheaper than managing an actual laboratory. Further, providing a visualization of the molecular structures with computer graphics can assist in easily understanding the concepts. As such, applying computational chemistry to the chemistry education field has many advantages. However, most chemistry classes often focus only on an introduction of computational chemistry rather than covering deeper topics owing to a lack of computing resources or trained teaching assistants. Further, laboratory exercises are also generally conducted as a simple project at the end of the semester[1]. To attract the participation of students, a computational chemistry environment that all students can easily access should be provided. Frequently used software programs in the engineering field such as CAD support simple operations in a PC environment, allowing students to easily practice using their own personal computers. However, in the case of computational chemistry software, the programs are generally implemented in Unix rather than Windows, and even if implemented for Windows OS, the

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license is usually too expensive for students to buy and install on their own PCs[2].

To implement a suitable computational science software, there is an issue in which a high-performance computing infrastructure should be constructed to allow a large number of users to solve and interpret problems using the computational science software. However, this can be addressed by providing a user-friendly web-based interface environment. For this reason, the Korea Institute of Science and Technology has developed and serviced a computational science platform called EDISON since 2011 and has offered the EDISON Computational Chemistry service since 2012[3,4]. Offered through the Science App, the EDISON Computational Chemistry is software that can analyze various chemical phenomena that occur in various scales ranging from an atomic size of 10^{-10} m to several millimeters (mm) and at various time scales ranging from femtoseconds (10^{-15} s) to hours[1]. However, most of the services currently offered on Science App use text files as input. If a user is unfamiliar with the constraints of the input file, the user may unintentionally create an incorrect file, which in turn will lead to incorrect interpretations of the analysis and results. In addition, the user may inconveniently be required to check the results locally on a PC using a separate visualization software because Science App does not support some of the required web-based visualization tools. Further, most visualization software titles are generally professional programs intended for researchers, and students may find difficulties in using them[5].

Based on the computational science platform, in this paper an online quantum chemistry experiment environment is introduced that can be used in numerous areas ranging from undergraduate chemistry education to expert research. The experiment environment was constructed using the simulation workbench and workflow, which are execution environments of Science App offered on the computational science platform. Further, a separate web-based input and output GUI interface was developed to enhance the usability. A three-dimensional molecular editor and a GUI for the parameter input were provided to enable the users to easily use the software. In addition, by providing a web-based visualization tool that can interpret and analyze various chemical phenomena such as molecular energies and orbitals, we constructed an online experiment environment in which the users can utilize quantum chemistry software without having to locally install separate visualization software on their PCs[6].

The remainder of this paper is constructed as follows. Chapter 2 introduces the related theory, and Chapter 3 describes the computational science platform and the main services used in this study. In Chapter 4, the components of the online experiment environment proposed in this study are described. Subsequently, Chapter 5 introduces example cases of the practical use of the proposed model. Chapter 6 compares the functions of the proposed system with other systems. Finally, Chapter 7 provides some concluding remarks.

2. Related research

2.1 Quantum chemistry software

Quantum chemistry software is widely used in computational chemistry to compute quantum chemistry tasks. Quantum chemistry software generally utilizes Hartree-Fock(HF), Post-Hartree-Fock, density functional theory (DFT), Molecular mechanics, and semi-empirical quantum chemistry methods, and is typically available in the form of open-source or commercial software. Table 1 summarizes the currently available state-of-the-art quantum chemistry software[7].

2.1.1 Gaussian

Developed by Gaussian, Inc. (USA), Gaussian[8]. is one of the most widely used software programs in the field of quantum chemistry. The software modeling package supports predicting energy levels, molecular structures, and vibrational frequencies, and is generally used by researchers in the fields of chemistry, physics, life sciences, and engineering. The two researchers who were instrumental in the development of Gaussian won a Nobel Prize in 1998 for their contribution to the development of a package providing a Gaussian dedicated GUI software called GaussView, which mostly uses text-based input and output. The GUI supports constructing molecular systems of various inputs and can graphically display various results such as vibrational frequencies, molecular orbitals, NMR, and UV-Vis spectrum

(Table 1) List of quantum chemistry and solid-state physics software

Package	License	Academic Prices	GUI SW	Language	Basis	Periodic	Support Method			
							Semi-emp	HF	Post-HF	DFT
Gaussian[8]	Commercial	$35,000	GaussView($6,000)	Fortran	GTO	Any	Yes	Yes	Yes	Yes
Jaguar[9]	Commercial	$5,000/ year	MAESTRO(free for non-commercial use)	Fortran, C	GTO	No	No	Yes	Yes	Yes
Q-Chem[10]	Academic, Commercial	$3,899	IQMol(Free)	Fortran, C, C++	GTO	No	Yes	Yes	Yes	Yes
GAMESS(US) [11]	Academic	Free	MOLDEN, Facio, WebMO	Fortran, C	GTO	No	Yes	Yes	Yes	Yes
ACE-Molecule [12]	Free, GPL	Free	No	C++	Grid, Lagrange func.	Any	Yes	No	Yes	Yes

2.1.2 Jaguar

Developed by Schrodinger (USA), Jaguar[9] is a quantum chemistry software that provides a high-performance ab initio electronic structure interpretation. Jaguar provides a GUI called Maestro, which is free to use for academic and non-commercial use.

2.1.3 Q-Chem

Developed by Q-Chem[10], Inc. (USA), Q-Chem is a first-principle quantum chemistry software package that supports accurate predictions of molecular structures, reactivities, and vibrational, electronic, and NMR spectra. The latest release of Q-Chem supports high-performance DFT/HF calculations and high-level post-HF correlation calculation methods. Q-Chem also supports using both wave function-based methods and density functional theory, and comes with a graphical user interface called IQmol, which is a free GUI developed by Andrew Gilbert of Australian National University.

2.1.4 GAMESS

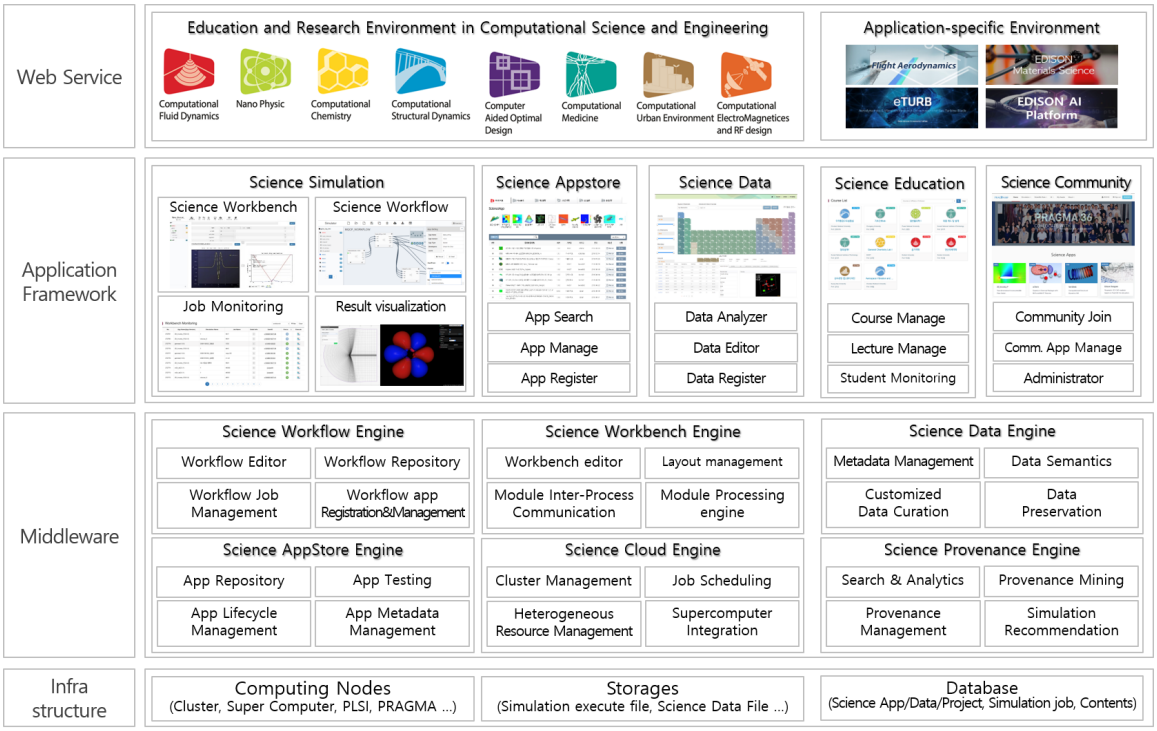
GAMESS (US)[11] is a computer software program for computational chemistry programs. Its development started in 1977, and in 1981, the project was split into GAMESS (USA) and GAMESS (UK). GAMESS (USA) is maintained by the members of the Gordon Research Group at Iowa State University, and it currently has approximately 150,000 users in over 100 countries throughout the world.

2.1.5 ACE-Molecule

ACE-Molecule is an open-source quantum chemistry software developed in Korea. Developed by researchers at the Korea Institute of Science and Technology, ACE-Molecule software adopts a new grid-based function based on the existing Gaussian function calculation code. The software is aimed at providing more accurate and faster electronic structure calculations for large molecular systems. The main features currently offered include ground-state DFT calculations using LDA and GGA, KLI approximation, and atomic force calculations using a linear-response TD-DFT, CIS, and CISD methods[12].

2.2 Web-based Quantum Chemistry Simulation Service

WebMO[13] is a popular web-based service that provides web-based computational quantum chemistry software. WebMO is simply a web-based interface service for computational chemistry packages available to students and non-specialists. WebMO provides easy input access not only to intermediate users but also to beginners without much difficulty, and provides a suitable GUI environment for conducting calculations and checking and analyzing the results. In addition, WebMo features support for most popular quantum chemistry software packages such as Gamess and Gaussian, and supports all modern web browsers (e.g., Edge, Explorer, Safari, Chrome, and Firefox) and iOS and Android devices, in turn, allowing easy access to



(Figure 1) Architecture of computational science platform and major web services

quantum chemistry software from any device. WebMO features Basic, Pro, and Enterprise versions, and WebMo Basic can be downloaded for free. On the web, the Basic version can only be used as a type of trial version, and to use the graphical visualization features such as electron density and molecular orbitals, the Pro version needs to be purchased and installed.

3. Computational Science Platform

To provide an environment in which users can easily access computational science software through the web, KISTI has developed and is servicing a computational science platform (EDISON). Currently, the platform is featuring services in eight different fields and has secured over 70,000 users in Korea. The computational science platform is mainly composed of three layers: an application framework, middleware, and infrastructure. The overall structure of the computational science platform is shown in Figure 1. The application framework is implemented based on Liferay Portal[14], which is an enterprise portal solution. Some of the popular services provided by Liferay include a workbench service in a single application execution environment, a workflow service that allows designing and executing simulations, a simulation data service that allows storing and sharing large-scale simulation data, and a science application store that allows registering and managing various simulation software. The middleware layer supports various core platform management functions such as metadata management for Science App services, simulation dataset management, simulation history management, science workflow management, user authentication and authorization management, and heterogeneous (virtual and physical) computing resource management. Finally, the infrastructure layer is designed to support large-scale computing and input and output for simulation tasks executed by users. The infrastructure layer is composed of a total of 1,752 physical cores supporting up to 14.4 teraflops[15].

3.1 Workbench

The workbench provides an environment for executing a single Science App, and supports the general computational science software execution steps of pre-processing, execution, and post-processing. The workbench screen is divided into menu, task, and layout areas. The menu area lists the functions necessary for executing the simulation, and the task area provides the function of managing the simulation task. Finally, the layout area displays the editor and analyzer used to execute the application[6,16].

3.2 Workflow

By using the applications registered on the platform, the workflow enables an efficient execution by automating the execution according to the flow defined by the user. The constructed workflow can be registered as a new separate application and is sharable with other users. The workflow provides reuse, pause, and re-execute functions of the workflow, and its usability is enhanced by providing the controller and converter modules[6].

4. Constructing an Online Quantum Chemistry Experiment Environment

To construct an effective quantum computing software-based online experiment environment, the following requirements should be fulfilled. First, high-quality quantum chemistry software should be used. To fulfill this, we used the ACE-Molecule package, which is a quantum chemistry software package developed at KAIST. Second, an easy and convenient interface should be provided to the users. For this reason, we acquired requirements for the interface improvements from the ACE-Molecule developers and designed an interface suitable for the software. Third, an interactive experiment environment should be supported to induce user interest in learning. To achieve this, we implemented workflows in some of the experiment content to allow users to easily grasp the meaning of an experiment by simply constructing a simulation. Finally, meaningful content that the users can find interest in should be designed and provided. As such, we selected experiment topics that can be implemented in various chemistry fields such as general chemistry, physical chemistry, and computational chemistry, and constructed theoretical learning materials in the form of e-learning content[22].

(Table 2) List of quantum chemistry SW

SW	Description
ACE-molecule (17)	TD-DFT, CIS, and CISD methods are used to perform accurate and fast electronic structural calculations for large molecular systems.
ACE_UV_analysis (18)	Calculate UV spectrum of TDDFT calculation result of ACE-Molecule.
K-EHT(19)	Calculate molecular energy, molecular orbital and orbital energy using the extended Hückel theory
tdLagChem(20)	Using the time-dependent Schrödinger equation, calculate the wave function of a single particle for a 1D potential
LagChem(21)	Using the Schrödinger equation, calculate the wave function of a single particle for a 1D potential

4.1 Quantum Chemistry Software

To construct an online quantum chemistry experiment environment, Science App, which is offered by the EDISON computational chemistry webpage, was used. Table 2 summarizes the Science App used in this study.

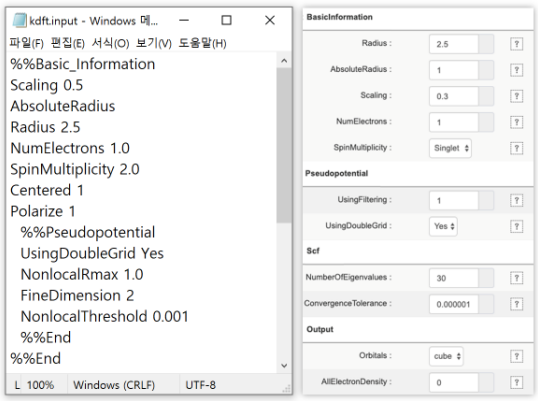
4.2 Web-based Input Data Editor

Most computational scientists generally use text editors to construct input parameters and special tools to generate input data of complex structures (e.g., molecular and protein structures). Thus, beginners often fail to understand the different parameter input rules for each computational software, which may often lead to a malfunction or errors in the results. To address this issue, the computational science platform provides a Structured Data Editor (SDE) that can be used to create a parameter input, and a general-purpose 3-D molecular editor that can be used in the computational chemistry software.

4.2.1 Structured Data Editor(SDE)

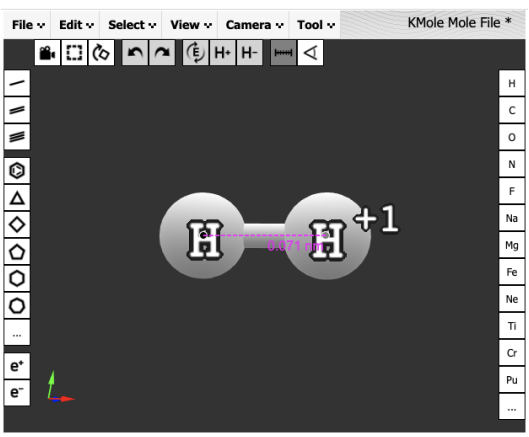
When requiring a parameter input file among the Science App input files, a user can simply configure a web-based GUI to enter the parameters using the SDE tool. In the GUI

screen, the rules for the input file can be specified, and the required parameters can be constructed. Figure 2 (a) shows the text input of ACE-Molecule, and Figure 2 (b) shows the parameter input GUI implementation of ACE-Molecule using the SDE tool.



(a) Text Input (b) SDE Input

(Figure 2) Compare Text Input and SDE Input



(Figure 3) Web-based 3D molecular editor(KMol)

4.2.2 KMol

KMol is a web-based 3-D molecular editor, which supports various data formats used in computational chemistry such as MOL, XYZ, PDB, CML, CIF, and POSCAR. Figure 3 shows the execution screenshot of KMol. The KMol editor allows placing chemical elements in any desired space and adding chemical bonds. The editor also enables users to easily select the desired elements by placing the frequently used chemical elements on the left side of the screen. Further, it allows the users to select elements from the periodic table and add predefined molecules such as benzene rings. In addition, the KMol editor provides features for optimizing the chemical bond angle and bond calculation of a simple molecular structure, as well as for adding or removing hydrogen and electrons.

4.3 Web-based Result Data Analyzer

In constructing the quantum chemistry experiment environment, various visualization tools were used to display the execution results. We developed an Orbital Viewer to support the display of one type of analysis results, i.e., molecular orbitals.

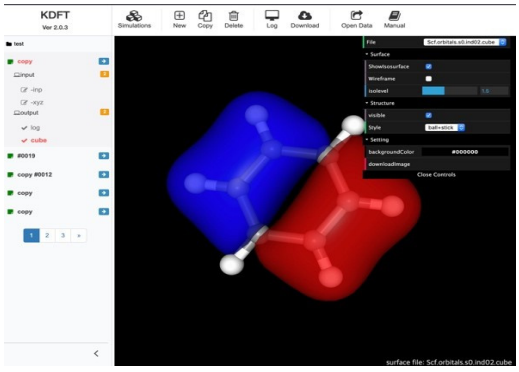
4.3.1 Web-based 3D Molecular Orbital Visualizer

Orbital Viewer was designed to display the 3-D structure of the molecular orbitals obtained from the analysis results of ACE-Molecule and K-EHT. In terms of visualizing the results of quantum chemistry, the existing analyzers of the computational science platform support various tools such as NGL Viewer[23] and JSmol Viewer[24]. However, the NGL Viewer was developed as a general-purpose viewer and supports molecular orbital visualization, although the default isolevel is too high, requiring the user to manually adjust it to check the orbitals. Further, the positive and negative values must be visualized in different colors when observing the orbital phase, although the NGL Viewer tool requires the user to manually set the configurations such as the adding surface. In the case of the JSmol Viewer, although the visualization of the position of the atomic nucleus of the molecules is supported, it does not support molecular orbital visualization. We developed the Orbital Viewer tool to solve such issues.

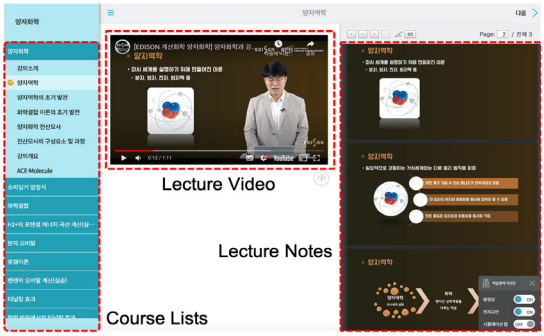
Orbital Viewer supports reading a cube file, which is one of the formats for storing volumetric data as well as the atom positions. Further, the viewer is designed to visualize the molecular orbital structure using the ngl.js library. Figure 4 displays the menu screen of the viewer tool. Here, a cube file can be selected from the simulation result files. Further, the viewer tool can be used to change the molecular structures

into various structures, view the surface with a wireframe, and adjust the isolevel. Figure 5 shows the execution screen of the viewer tool. Here, the proposed orbital viewer can be used to view the orbital structure, which is one of the resulting files.

(Figure 4) Menu of the Orbital Viewer



(Figure 5) Execution screen of the Orbital Viewer



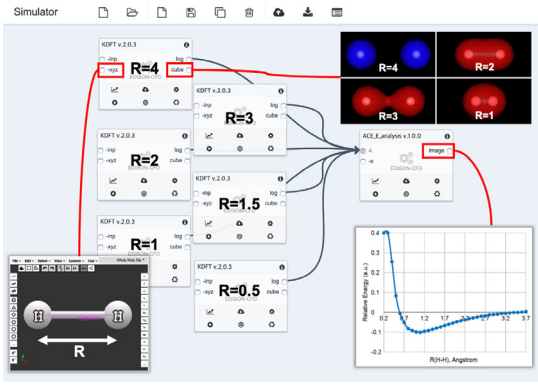
(Figure 6) Quantum chemistry MOOC contents

5. Use Cases

As shown in Figure 4, laboratory exercises were organized using the quantum chemistry software and web-based input and output tools discussed in Chapter 4. To help users easily understand the experiment contents, related theoretical materials were produced as images in the form of MOOC. Figure 6 shows the quantum chemistry MOOC offered by the EDISON computational chemistry platform[25].

5.1 Chemical Bond

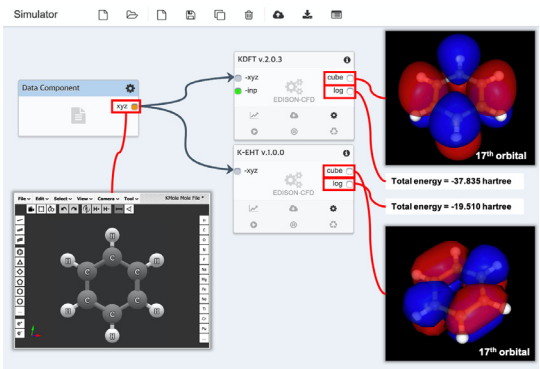
To help users easily grasp the chemical bond phenomenon of the molecules, we constructed an exercise for finding the potential energy according to the position of a H_2^+ molecule and graphing it through a simulation. For this process, the ACE-Molecule package was used, and as shown in Figure 7, the experiment environment was constructed using the workflow. The workflow consists of finding the potential energy for each molecule position and drawing the potential energy obtained on a graph. As shown in the figure, the first step enables examining the distribution of the potential energy and orbital according to the molecule positions. In addition, the second step allows analyzing the potential energy curve of the H_2^+ molecule. Through this use example, the user can understand the principles of chemical bonds and the Born-Oppenheimer approximation theory.



(Figure 7) Use Cases : Chemical Bond

(Table 3) List of quantum chemistry education contents for online experiment environment

Title	Main theory explanation	Virtual experiment contents	Software
Quantum mechanics and chemical bonding	Schrodinger's Equation and Chemical Bonding	Calculate the potential energy curve for H_2^+	ACE-molecule
Molecular orbital	Molecular orbital Hückel method	Orbital calculation of benzene	K-EHT, ACE-molecule
Tunneling effect	Tunneling effect and time-independent/dependent Schrodinger equation in chemical reactions	Nitrogen inversion barrier energy calculation and tunneling effect	ACE-molecule, tdLagChem, LagChem
UV-visible spectroscopy	Molecular energy state and excited state, UV-visible spectroscopy	UV-visible light absorption spectrum calculation	ACE-molecule, ACE_UV_analysis



(Figure 8) Use Cases : Molecular Orbital

5.2 Molecular Orbital

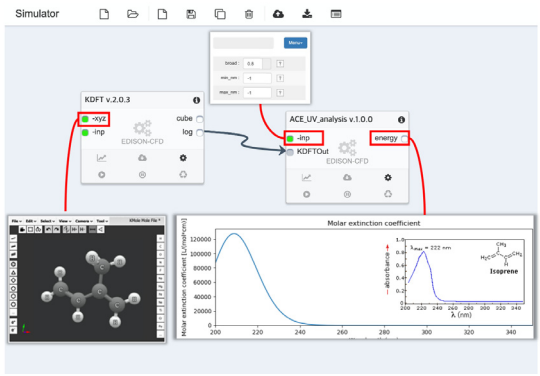
To help the users understand the molecular orbitals (MO), we constructed an exercise for calculating the orbital energy and structure of benzene using the extended Hückel theory (EHT) and density function theory (DFT). Because obtaining an accurate wave function for molecules other than H_2^+ molecules is impossible, the molecular orbitals can be obtained based on a linear combination of the atomic orbitals through the linear combination of atomic orbitals method (LCAO-MO method). As shown in Figure 8, the environment of the laboratory experiment was designed in such a way that users can compare and analyze multiple methods through the workflow.

5.3 Quantum Tunneling

Quantum tunneling, or simply tunneling, refers to a quantum mechanical phenomenon in which the nucleon constituting the atomic nucleus has a finite probability of crossing an energy barrier even when its energy is less than the potential energy barrier. Through this property, the radioactive decay of the nucleus can be described, and a scanning tunneling microscope equipment capable of obtaining atomic-level surface images can be developed. Through experiments, the user can understand nitrogen inversion, which is a phenomenon in which a pyramidal molecule generated from a nitrogen compound turns inside out. The energy barrier can be obtained through the ACE-Molecule package, and the wavefunction for each energy can be obtained using the time-independent Schrödinger equation (TISE) from LagChem software. Finally, a change in the wavefunction over time can be observed using the time-dependent Schrödinger equation (TDSE) from tdLagChem software.

5.4 UV-Visible Spectroscopy

A molecular electronic transition occurs when atoms and molecules in the ground state absorb ultraviolet and visible light. Depending on the type of atom or molecule, the characteristics of the absorbing light of a specific wavelength varies, and based on the absorbed wavelength, the type of atom or molecule can be determined. Figure 9 shows the experiment environment of the UV absorption curve of Isoprene using the workflow. The ACE-Molecule package can be used to calculate the electronic structure of the molecule's ground state based on the TDDFT, and ACE_UV_analysis can be used to examine the graph of the absorbance curve. The use of TDDFT enables the electron excitation states of the molecules to be calculated more quickly and accurately than other methods. Further, this method also allows replacing the expensive UV-VIS spectrophotometer used in different experiments.



(Figure 9) Use Cases : UV-Visible Spectroscopy

(Table 4) Compare web-based quantum chemical simulation services

Item	WebMO		Proposed system
	Basic	Pro	
3D molecular editor & viewer	Support		Support
UV-VIS spectra	Support		Support
Visualization of molecular orbitals	Not Support	Support	Support
Software	Gaussian, Gamess etc.		ACE-Molecule etc.
Type of Service	Cloud	Install on a your PC	Cloud
Job's time limit	1 min	No limit	120 Hours
Number of cores per user	1 Core	No limit	8 Cores
License Prices (Academic)	Free	$995	Free
E-learning Contents	Not Support		Support
Workflow	Not Support		Support

6. Compare web-based quantum chemical simulation services

Table 4 shows a comparison between the proposed service developed through this study and a state-of-the-art web-based quantum chemistry simulation service. The proposed service provides most of the services and features provided in the WebMo Basic version, as well as a molecular orbital visualization feature, which is offered only in the WebMo Pro version. To fully utilize the functions of WebMO, a user must install WebMo on a personal computer and link it with the quantum chemistry software held by the user. Further, although WebMo provides a trial version on its webpage, it can only be used with a guest account, and each task execution time is also limited to a maximum of 1 minute. By contrast, because the service proposed through this study supports various environments from computational resources to a web-based execution environment, it can be directly used without requiring any additional installations. In addition, the proposed service provides computing resources for various research purposes by providing up to eight CPUs that can be used simultaneously and a maximum execution time of 120 h. In addition, the proposed service features a workflow, which is not provided by WebMo, and it enhances the user convenience by providing e-learning video content for the experiments.

7. Conclusions

This paper described an online experiment environment that can be used for various purposes ranging from basic education courses related to quantum chemistry to professional research. To establish such an environment, we used ACE-Molecule, an open-source quantum chemistry software package developed in Korea. Further, various web-based editors and analyzers were developed to provide a simple and easy-to-use interface to the users. In addition, using the workbench offered in the computational science platform, we constructed an experiment environment in which quantum chemistry simulations can be simply performed with Internet access, and through experiment examples, we also linked several quantum chemistry software programs through a workflow. In this way, we expect users to be able to structurally understand the operation of quantum chemistry software. Overall, we developed an environment in which students can learn independently without requiring an instructor by selecting experiment topics that can be used in various chemistry subjects and offering the learning materials of the topics in a form of e-learning content including theory and simulation exercises.

By providing a web-based educational and research simulation software application environment, our proposed

model is expected to contribute to the realization of a practice- and experiment-oriented teaching method through the proposed software and educational contents while breaking away from the existing theory-oriented teaching methods. In addition, our model can be implemented in a web-based higher education system to enable modern students familiar with IT to easily access the education system and utilize the virtual experiment environment. In this way, the proposed model is expected to induce learning motivation to the learners, and in turn, nurture advanced talents and resources in the field of computational chemistry and contribute to an enhancement of future national research talents.

참고문헌(Reference)

[1] Seokmin Shin, et al. “Development and Application of Simulation Software for Education and Research in Computational Chemistry”, Final Report, July 2017.

[2] Hoon Ryu, Junglok Yu, Du seok Jin, Jun-Hyung Lee, Dukyun Nam, Jong-Suk Ruth Lee, Kumwon Cho, Heejung Byun, and Ok-Hwan Byeon, “EDISON Science Gateway: A Cyber-Environment for Domain-Neutral Scientific Computing”, IEICE Transactions 97-D, Vol.8, pp.1953-1964, 2014.

[3] EDISON (EDucation-research Integration through Simulation On the Net, https://www.edison.re.kr)

[4] EDISON-CHEM (https://chem.edison.re.kr)

[5] Young Kyoon Suh, "Construction and Service of a Web-based Cyber-learning Platform for the Computational Science and Engineering Community in Korea", Journal of Internet Computing and Services Vol. 17, No. 4, pp. 115-126, Aug. 2016. https://doi.org/10.7472/jksii.2016.17.4.115

[6] Inho Jeon et al., "Construction and Service of a Web-based Simulation software management system for the Computational Science and Engineering", Journal of Internet Computing and Services Vol. 18, No. 4, pp. 99-108, Aug. 2017. https://doi.org/10.7472/jksii.2017.18.4.99

[7] Wikipedia, s.v. "List of quantum chemistry and solid-state physics software" last modified May 29, https://en.wikipedia.org/wiki/List_of_quantum_chemistry_and_solid-state_physics_software

[8] Gaussian, https://gaussian.com

[9] Jaguar, https://www.schrodinger.com/jaguar

[10] Q-Chem, www.q-chem.com

[11] GAMESS, https://www.msg.chem.iastate.edu/gamess

[12] ACE-Molecule, https://gitlab.com/aceteam.kaist/ACE-Molecule

[13] WebMO, https://www.webmo.net

[14] Liferay, http://www.liferay.com

[15] Jongsuk R. Lee, et al. “Research and Development (R&D) of the EDISON (EDucation-research Integration through Simulation On the Net) platform and Its User Service on Cyber-Infrastructure”, Report of the 2nd (overall 9th) year R&D in the 4th phase, January 2020.

[16] Kwon, Yejin, et al. “Interface Development for Pre and Post processor on EDISON Platform Simulation System.” Journal of Internet Computing and Services Vol. 21, No. 1, pp. 103 – 110, Feb. 2020, https://doi.org/10.7472/jksii.2016.17.4.115

[17] ACE-Molecule, EDISON SW, https://www.edison.re.kr/scienceappstore/- /scienceapp/KDFT/2-0-3/view

[18] ACE_UV_analysis, EDISON SW, https://www.edison.re.kr/scienceappstore/-/scienceapp/ACE_UV_analysis/1-0-0/view

[19] K-EHT, EDISON SW, https://www.edison.re.kr/scienceappstore/-/scienceapp/K-EHT/1-0-0/view

[20] tdLagChem, EDISON SW, https://www.edison.re.kr/scienceappstore/-/scienceapp/tdLagChem/1-0-0/view

[21] LagChem, EDISON SW, https://www.edison.re.kr/scienceappstore/-/scienceapp/LagChem/1-0-0/view

[22] Shin, Jung-Hun, et al."Workflow-based Environment and its Use Scenario for the Education of Connective Engineering Simulation", Journal of Engineering Education Research, Vol. 21, Issue 6, pp. 3-12, Nov. 2018

[23] Ngl.js, https://github.com/arose/ngl

[24] JSMol, http://jmol.sourceforge.net

[25] EDISON CHEM e-learning, https://elearning.edison.re.kr/chem

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