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The Extension of Monomeric Computational Results to Polymeric Measurable Properties: An Introductory Computational Chemistry Experiment

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***Abstract*—**Advances in software technology enable the computational chemistry to be commonly applied in various research fields, especially in pedagogy. Thus, in order to expand and improve experimental instructions of computational chemistry for undergraduates, we designed an introductory experiment—research on acrylamide molecular structure and physicochemical properties. Initially, students construct molecular models of acrylamide and polyacrylamide in Gaussian and Materials Studio software respectively. Then, the infrared spectral data, atomic charge and molecular orbitals of acrylamide as well as solvation effect of polyacrylamide are calculated to predict their physicochemical performance. At last, rheological experiments are used to validate these predictions. Through the combination of molecular simulation (performed on Gaussian, Materials Studio) with experimental verification (rheology experiment), learners have deeply comprehended the chemical nature of acrylamide and polyacrylamide, achieving good learning outcomes.

***Keywords*—**Upper-division undergraduate, computer-based learning, laboratory instruction, amides, molecular modeling, spectroscopy.

I. Introduction

COMPUTATIONAL chemistry is a core chemical discipline based on quantum chemistry and statistical mechanics with first principles as its fundamental approach.[1]-[3] After decades of development, it has made great success in both basic theory and practical application, acquiring massive achievements in chemistry, materials science, life science and other fields [4], [5]. For example: In colloidal chemistry, after establishing suitable models or preassembled structures, the size, shape, structure and surface strength of colloidal aggregates can be achieved by computational simulation of molecular motion within nanoseconds [6]. Thus, helpful guidance for colloidal chemistry experiment can be provided to clarify some complex reaction mechanisms. Therefore, with the rapid development of science and technology, the computational chemistry is increasingly demanded in a variety of research fields. Especially, the advanced computer science drastically prompts its popularization among college students [7]. In fact, the practical necessity of students using computational chemistry to explain reaction mechanisms and intermolecular interactions is fast growing. However, for lack of theoretical and operational foundation, self-learning outcome is always dissatisfied among students [8]. To meet the requirements for computational chemistry instruction, the universities in China have established a series of interwoven curricula. In Shandong University, the basic theory of molecular simulation has been designated for master-degree and doctoral candidates since 2003 [9], [10]. Again, since 2016, Yangzhou University has made modern molecular simulation technology as an elective course for postgraduate and doctoral students, achieving good pedagogical effectiveness. Also, researchers have designed and implemented a sequence of computational laboratory experiments for undergraduates, achieving excellent pedagogical effect [11], [12], [18]. Whisnant et al. constructed a computational lab exercise to calculate the vibrational spectra of various alkyne molecules in comparison with the experimental data [31], from which students extensively explored how molecular symmetry and structure affect vibrational spectra. Moreover, a computational experiment, proposed by Daniel et al., investigate molecular models for single-layer two-dimensional (2D) materials (hexagonal boron−carbon−nitrogen sheets), thus exemplifying the relationship of electronic properties and chemical structures of 2D materials [33]. Meanwhile, more and more researchers have integrated computational exercises into other chemistry lab curricula (such as physical chemistry and organic chemistry, etc.) for enhancing the theoretical instruction [1], [13]-[16]. Miller et al. introduced computational chemistry into the physicochemical experiment and obtained good instructional effects, during which the Spartan software was used to establish Walsh diagrams for predicting the bond angle of ground-state molecules and explaining the molecular orbital-structure relationship [13]. Again, Nassabeh et al. incorporated a set of computational exercises into a physical chemistry laboratory curriculum, and employed Gaussian 03W, WebMO and Jmol software to analyze the unimolecular dissociation of ethyl radical, acquiring superior synergistic effects [14]. However, the aforementioned curricular designs from universities and researchers mainly focused on the applications of computational chemistry, but few systematic introductions upon the theoretical foundation and basic software operations. As a result, it is difficult for learners to reasonably select the basis set and fully understand the calculation results, let alone the good self-instruction. Aiming at above problems, we intend to design an introductory experiment of computational chemistry: “research on molecular structure/physiochemical

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properties of acrylamide" for undergraduates majoring in polymer materials and engineering.

Compared with the previous researches, this experiment has the following advantages: 1) The instructions of basic structural chemistry theory, calculation principles and software operations are highlighted in this experiment, which is fairly helpful to leaners. 2) As a monomer commonly used in polymer synthesis, acrylamide molecule is quite representative and closely coincides with the professional background of learners [17]. Furthermore, the computational lab exercise can enhance the comprehension of structure-function connection, and acquire a good synergy with polymer chemistry lecture. 3) The integrative chain-like instructional sequence is conducive to students for constructing a rational thinking mode in computational chemistry research. The sequence includes: monomer molecular modeling—input file preparation—molecular configuration optimization—molecular vibration frequency calculation—molecular orbital and potential energy analysis—polymer model creation and optimization—solvation effect calculation—rheological experimental verification. 4) The combination of software simulation with experimental validation upgrades the awareness of theory-practice relationship in students, which is favorable for their academic careers.

II. Educational Context

The pedagogical foundation of this laboratory curriculum is the model and modeling framework proposed by Briggs. This theory is very useful in explanation molecular structure and chemical behaviors, thus offering the theoretical instruction [1], [10]. Specifically, the model consists of five parts: 1) referents, 2) relationships, 3) rules/syntax, 4) results and 5) operations (Fig. 1). The first four are static preconditions for illuminating the material nature, while the last one is the dynamic external changes exerted on material. Wherein, the referents are abstract symbols representing the research objectives; relationships are inherent connections among referents or between referents and environment; rules/syntax are the way how operations changing referents; operations are the external processes modifying referents, and results are the obtained products. The models and modeling framework theory can fully display the conceptual work of learners to help them construct a reasonable thinking mode. In fact, the models, established by learners, are their mental representations for research objectives. Besides, the modeling process requires indispensable knowledge accumulation on the research objectives. Therefore, the preview, guided by teachers, is of great importance for learning outcome (see pre-lab questions in supporting information).

Herein, the referent is acrylamide; relationships are its molecular structure and physicochemical properties; the rules/syntax are the physicochemical laws at microscale; operations refer to polymerization and stress-strain process; the results are polyacrylamide (PAM) and its aqueous solution (Fig. 1). Taking advantage of computational software (Gaussian, Materials Studio), the construction and visualization of the above model and modeling framework can be easily accomplished by learners. Various molecular movements and supramolecular actions can be simulated and calculated under different environments. Thus, it assists learners in comprehending the structure-function relationship of acrylamide and its theoretical models.

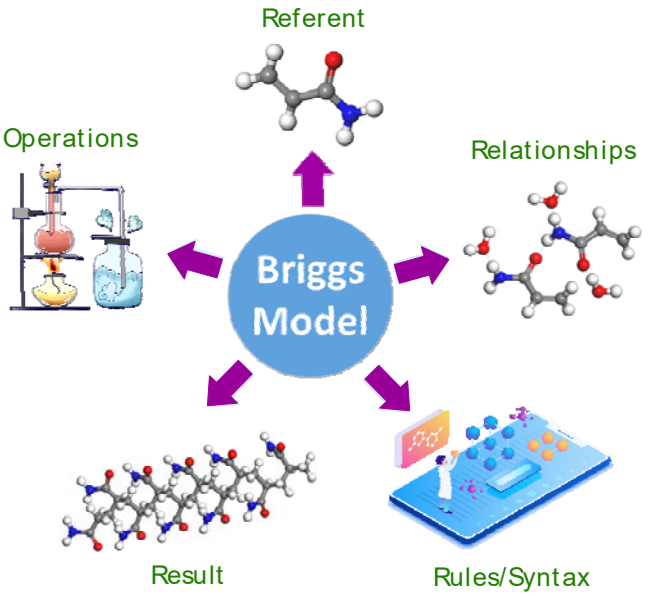

Fig. 1 Schematic illustration of theoretical framework

III. Experimental Section

A. Materials, Software and Equipment

Gaussian 09, GaussView 5.0 and Materials Studio 17.1 software were used in analog computation. Specifically, Guassian 09 and GaussView 5.0 were purchased from Gaussian Inc along with Materials Studio 17.1 from NeoTrident Technology Ltd. They were equipped in the departmental computer cluster running Win 7. Besides, many of the simulations in this work can also be performed on other software, such as Discovery Studio, Spartan and Accelyrs, etc. In addition, rheological experiments were conducted on DHR-2 rotary rheometer with the resultant data processed by TRIOS rheological analysis software in personal computer. Meanwhile, the nonionic PAM with a molecular weight of 5 million Da was provided by Macklin (China).

B. Experimental Procedure

Concerning the monomer-polymer system in this experiment coupled by the Briggs model theory, the main operational steps of computational simulation (Fig. 2) and experimental validation were as follows:

1. Monomer molecule modeling: A reasonable preliminary molecular configuration of acrylamide was drawn in GaussView by referring to the relative scientific monographs and research articles.
2. Selection of suitable algorithm and basis set: Directed by simulation targets and previous researches, the algorithm and basis set were tentatively determined, then adjusted according to the single point energy calculation results.
3. Vibration frequency calculation: The configuration

optimization, molecular orbital and electrostatic potential calculations were conducted by Gaussian 09 for acrylamide molecule model.

4. Polymer modeling: The molecular model of PAM was built in Materials Studio along with its configuration optimization.
5. Solvation effect computation: In aqueous environment, the supramolecular behaviors of PAM were simulated and calculated by Amorphous Cell module in Materials Studio.
6. Rheological experimental verification: Rheological measurement was implemented on a DHR-2 rotary rheometer to determine the viscoelastic modulus and viscosity of PAM aqueous solution. Consequently, the computational results and the structure-function relationship of PAM were verified and analyzed, respectively.
7. Record, collation and analysis of the computational results and experimental data.

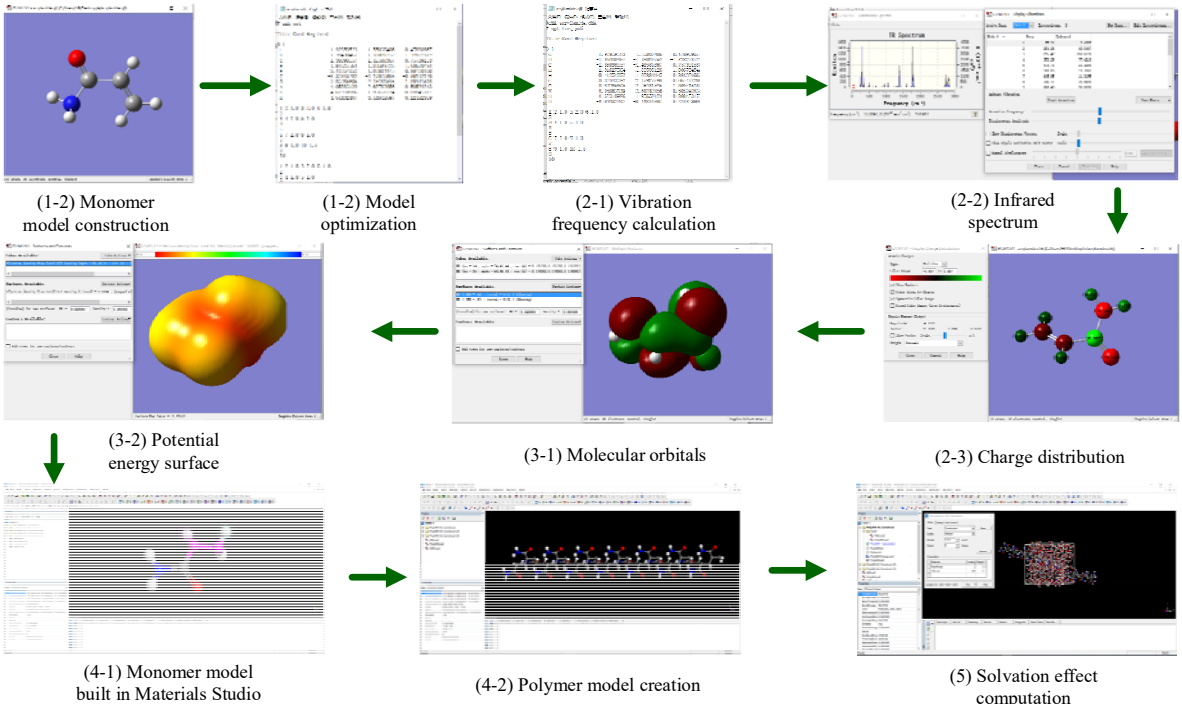

Fig. 2 Operation sequence of analog computation

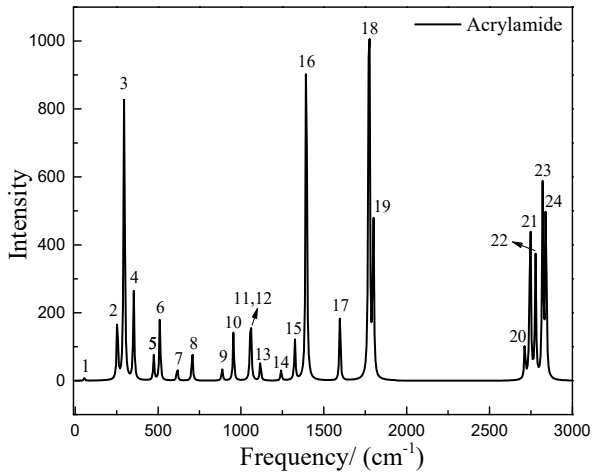

Fig. 3 Infrared spectrum of acrylamide

TABLE I
INFRARED SPECTRAL PEAK DATA OF ACRYLAMIDE

Peak number	Frequency/ (cm^{-1})	Intensity	Peak number	Frequency/ (cm^{-1})	Intensity
1	55.21	2.4207	13	1117.67	17.0232
2	254.28	60.0497	14	1242.93	8.8365
3	295.42	268.6270	15	1325.16	35.4492
4	353.29	77.4218	16	1394.42	356.6874
5	473.71	21.3293	17	1597.67	62.0668
6	510.85	53.7667	18	1773.10	436.8425
7	615.85	11.3159	19	1798.23	154.3830
8	706.12	26.9426	20	2713.42	29.6558
9	886.49	10.8638	21	2745.77	162.2933
10	955.06	43.6712	22	2777.53	104.8843
11	1054.75	16.7345	23	2820.42	164.2151
12	1059.99	51.0968	24	2839.88	164.9333

C. Hazards

The majority of this lab exercise was conducted by computer software, thus having great safety. Moreover, in regard to PAM aqueous solution preparation, it should be noted that it is harmful if swallowed.

IV. Results and Discussion

A. Computational Results

From the vibration frequency calculation, the single point energy, molecular orbitals and infrared spectrum data of acrylamide were obtained and displayed in Table I and Fig. 3. Simultaneously, the highest occupied molecular orbital

(HOMO), lowest unoccupied molecular orbital (LUMO), atomic charge and electrostatic potential surface were visualized and presented on the molecule in GaussView (Figs. 4 and 5). Besides, solvation effects of different PAM aqueous solutions were calculated and shown in Fig. 6.

According to Fig. 3 and Table I, the C=O and C-N stretching vibration bands have the highest intensity in infrared spectrum, indicating the most chemically-active amide group in acrylamide under infrared excitation [18], [19]. Furthermore, from Fig. 5, the overall electrostatic potential of acrylamide presents strong electronegativity. Herein, both the highest electron density and negative potential belong to the oxygen and nitrogen atom of amide group surrounded by HOMO and LUMO, while the highest positive charge density responses to the carbon atom in the same group (Fig. 4). The results indicate that as a powerful hydrogen-bond donor and acceptor synchronously [20], the amide group is of substantially high chemical reactivity in acrylamide, and can combine with homologous molecules or other hydrogen-bond donors/ acceptors to form robust supramolecular connections [21].

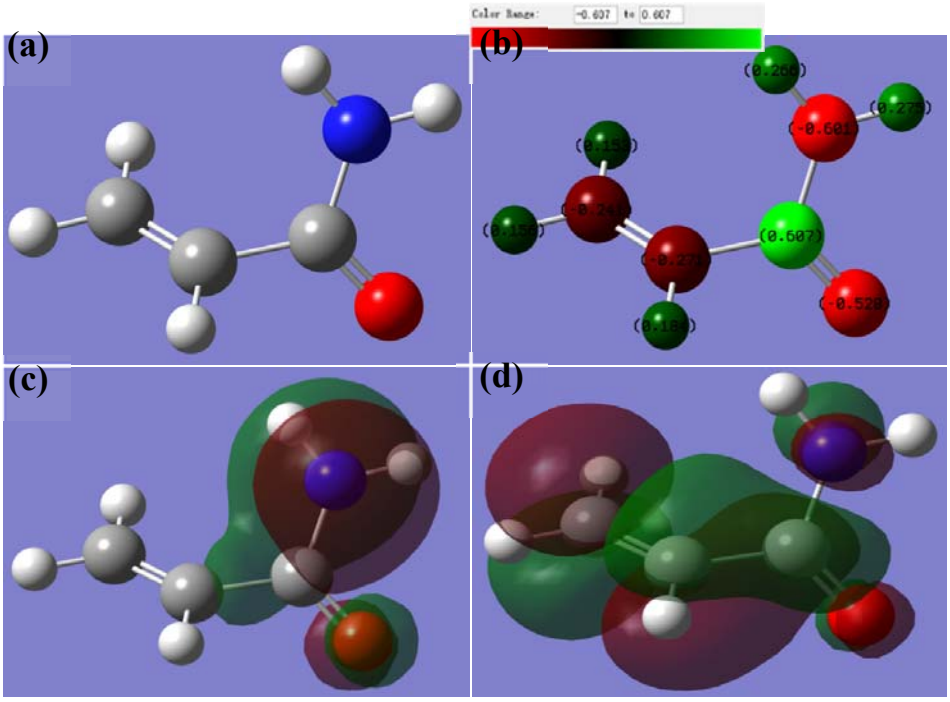

Fig. 4 Acrylamide: (a) Molecule configuration, (b) Charge distribution (Color range: -0.607~0.607 a. u. from red to green), (c) HOMO, (d) LUMO

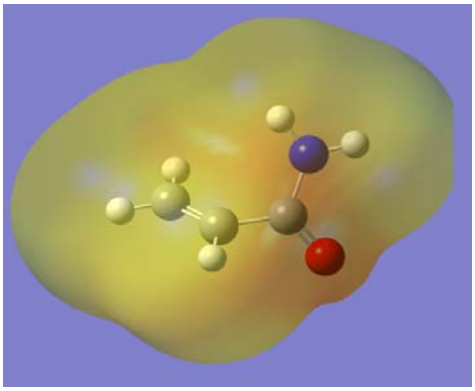

Fig. 5 Electrostatic potential distribution of acrylamide (Color range: -3.000~3.000 a.u.)

From Fig. 6, PAM molecules were evenly dispersed into water molecules. When the molar ratio of PAM : H_2O was 2 : 100, water molecules aggregated around PAM and distributed along polymer chain, indicating the strong affinity of PAM to water. Therefore, PAM can form massive hydrogen bonds with water molecules, so as to restrict its motion [22]. Again, compared with model 1, the solution system in model 2 has higher energy derived from more supramolecular connections between PAM chains. Obviously, the PAM is more liable to form hydrogen-bond connections with water molecules than the homologous molecules for reducing system energy, which is conducive to water locking [23], [24].

B. Rheological Experimental Validation

Frequency and flow sweep of 0.5 wt% PAM aqueous solution were conducted on a rotary rheometer to determine its viscoelastic properties and verify the analog computation outcomes. The results were displayed in Fig. 7.

In Fig. 7, at low shear rate, PAM dilute solution had large storage modulus (13.4 Pa at 1 s^{-1}) and viscosity (38.7 Pa·s at 1 s^{-1}) with its average loss factor 0.259 (tanδ, tanδ = G''/G') far below 1, suggesting its weak fluidity, high strength and solid-like property. Clearly, the chemically active amide groups endow PAM with good electronic supply and reception ability. Therefore, in a protic solvent (such as water), PAM tends to integrate with solvent molecules via supramolecular

interactions instead of the homologous molecules [25], [26]. This characteristic makes PAM solidly bind the solvent molecules to reduce their freedom degree, thus declining the solution liquidity and enhancing the viscosity [27].

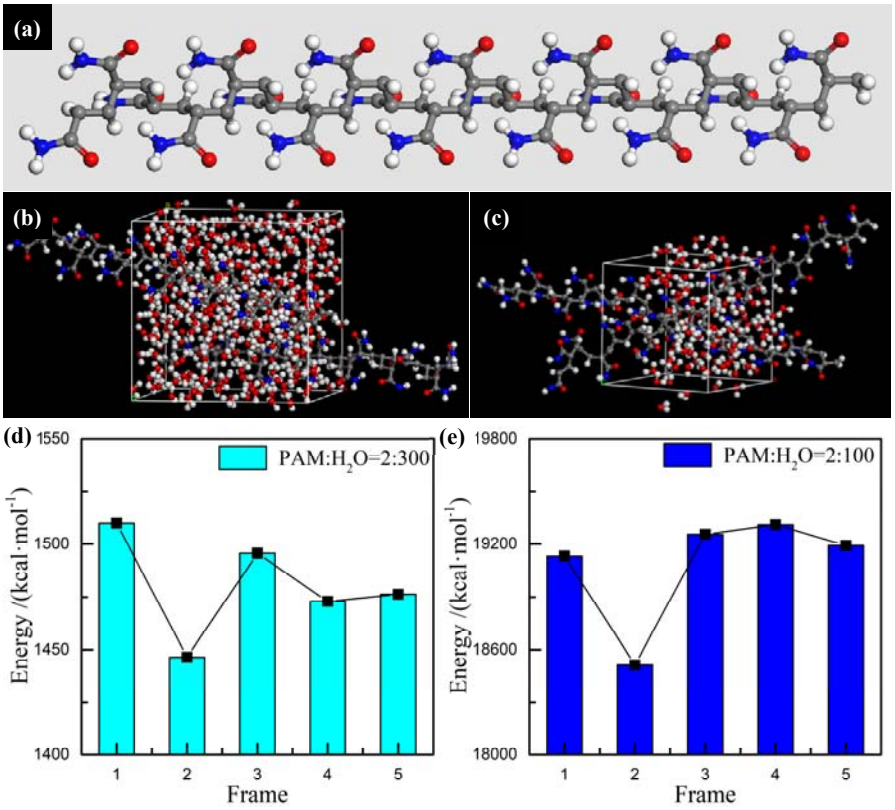

Fig. 6 PAM: (a) Molecular configuration, (b) and (d) Aqueous solution model 1 (PAM : H_2O = 2 : 300) and its energy-frame curve, (c) and (e) Aqueous solution model 2 (PAM : H_2O = 2 : 100) and its energy-frame curve

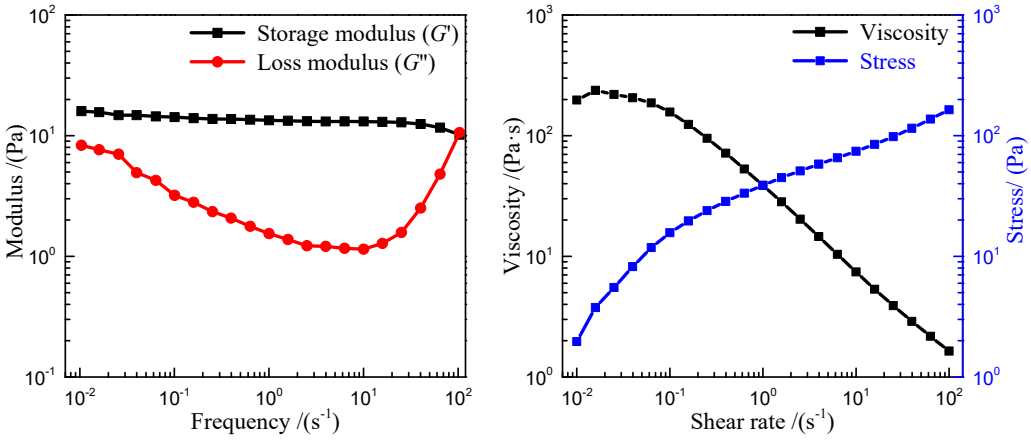

Fig. 7 Rheological properties of PAM aqueous solution: (a) Frequency sweep results, (b) Flow sweep results

V. Assessment

By means of questionnaire, interview, lab report (see supporting information) and written examination, the formative assessment was employed to evaluate the learning outcomes and analyze the curricular practicability, expansibility and limitations. Concretely, the evaluation was divided into two stages: 1) pre-tests (see supporting information) and 2) post-lab examination/tracking survey. Wherein, the pre-tests were performed on all participants in the laboratory experiment to test their preview results. While after class, the instructional outcomes and curricular limitations (Fig. 8) were analyzed on the basis of test results and lab reports of learners. Meanwhile, through questionnaires and interviews, a series of tracking surveys was initiated on 5~10 randomly chosen learners to evaluate the curricular practicability (Figs. 9 (a)-(c)). Furthermore, as for the curricular expansibility, the citation and application of this experimental design were surveyed and

recorded as well (Fig. 9 (d)).

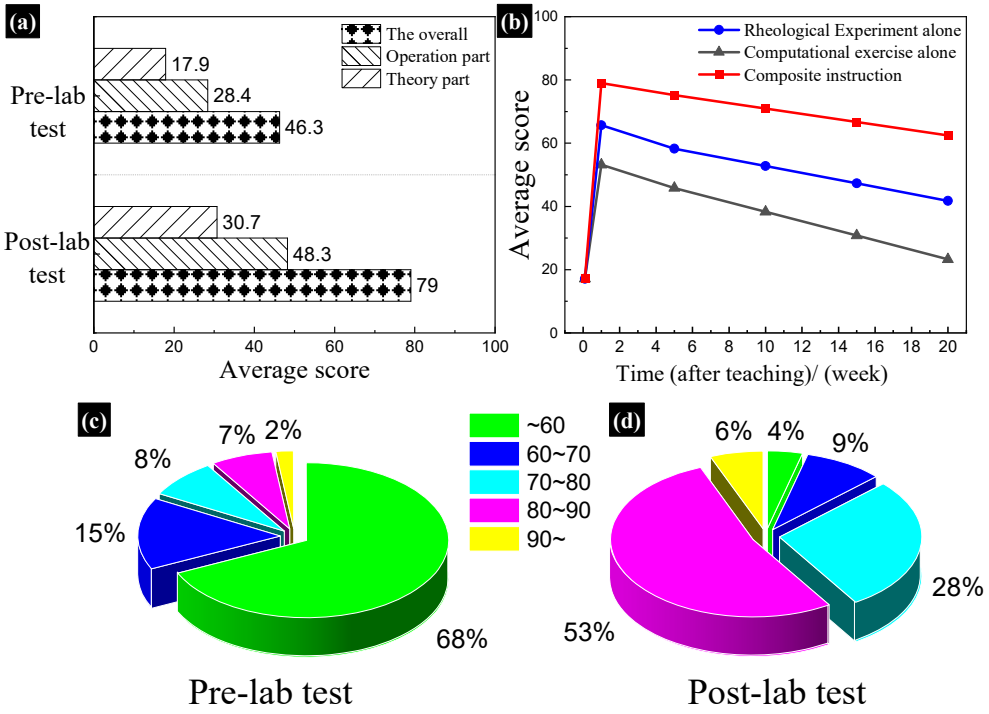

Fig. 8 Results of pre- and post-lab test: (a) Average score of pre- and post-lab test, (b) Average score of students who accept simulation exercise alone, rheological experiment alone and composite instruction, (c) and (d) Score distribution of pre- and post-lab test

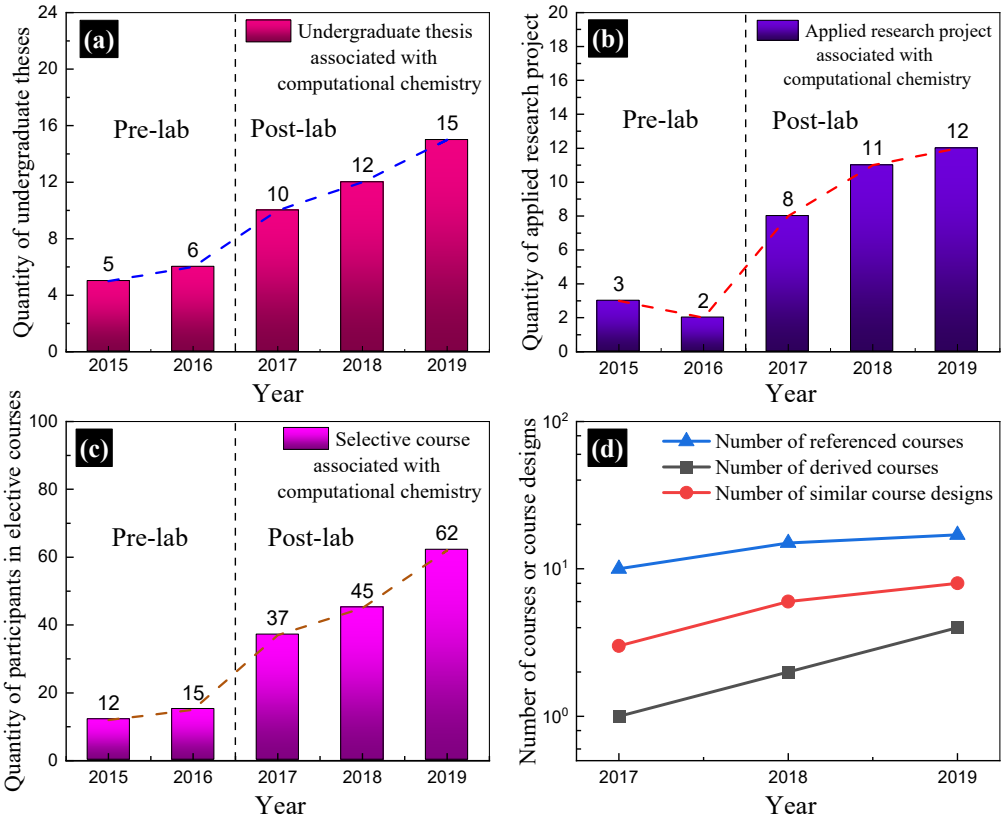

Fig. 9 Post-lab tracking survey results: (a) Quantity of computation chemistry-related undergraduate theses, (b) research projects and (c) elective course participants versus year, (d) experimental expansibility survey results

Based on Fig. 8 (a), after the experiment, the average scores of theory (score percentage: 50%), software operation (score percentage: 50%) and the overall in test were increased by 72%, 70% and 71% separately. Meanwhile, most learners scored 0% ~60% in pre-lab test and 80%~90% in post-lab (Figs. 8 (c) and (d)), demonstrating that the combination of theoretical and experimental instruction can remarkably enhance the pedagogical effectiveness. Additionally, according to the long-term tracking survey (Fig. 8 (b)), the average score was reduced gradually with time, while the compound instructional mode substantially enlarged the average score and knowledge retention in comparison to the single mode. In general, this lab exercise has engaged the learners in high-level thinking practices of computational chemistry and helped them master the basic operations of computational software [28]. Furthermore, the integration of computational simulation with experimental verification can notably elevate learners' awareness level on the structure-function relationship [28], [29].

Also, in Figs. 9 (a)-(c), as this laboratory curriculum implemented, the quantity of undergraduate theses and research projects involved with computational chemistry increased by 67% and 300% with more elective course participants (increment: 147%). Obviously, this experiment has effectively motivated and assisted students to further study computational chemistry. In addition, the application of computational software into other lectures (especially physical chemistry courses) was evidently enlarged as the software was more popular in public computers. Moreover, from Fig. 9 (d), the derived courses, similar curricular designs and citation frequency of this experiment have steadily grown with time, evidencing the enhanced interest in computational chemistry among teachers. From the aforementioned, this experiment efficiently enhanced the practical application of computational chemistry in learners and showed its great pedagogical potential to instructors [30]-[32].

VI. Conclusions

This laboratory experiment has integrated molecular simulation with hands-on rheological analysis to illustrate many introductory concepts and techniques of computational chemistry. Throughout the laboratory curriculum, students need to calculate various physicochemical parameters of acrylamide by computational software (Gaussian, Materials Studio) to predict and explain the supramolecular interactions in PAM aqueous solution. Meanwhile, they are also required to perform rheological experiments to determine the viscoelastic properties of the solution, thus verifying the simulation results. Comparing computational outcomes with experimental results, students' comprehension on polymeric supramolecular chemistry has been effectively deepened. Verified by the questionnaires, lab reports and written examinations, most students displayed good proficiency in software operations and hands-on experiment, and their interest in further studying computational chemistry was greatly motivated. On the other hand, the instructors also showed a high enthusiasm on the pedagogical application of computational chemistry by this experiment practice, suggesting its superior expandability.

Supporting Information

The supporting information includes: Student handout, instructor notes, pre-lab questions, lab report, supplemental tables (DOCX).

Ethical Statement

All procedures performed in studies involving human participants were in accordance with the ethical standards of the institutional and/or national research committee (Inst. IRB-FY2016-520) and with the 1964 Helsinki declaration and its later amendments or comparable ethical standards.

Consent Statement

Consent forms were collected from all the participants of this study.

Acknowledgments

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