Using Molecular Workbench in a Collaborative Discovery Learning Environment to Improve Students' Activities and Critical Thinking Abilities in Chemical Equilibrium

Andrian Saputra*, Lisa Tania, and Ila Rosilawati

***Abstract*—This study aimed to determine the effect of computer simulation using molecular workbench in a collaborative discovery learning environment to improve critical thinking abilities and learning activities of high school students. A quasi-experiment with a matching-only pretest-posttest control group design was applied in this study. A total of 60 students consisting of 30 students in both the experimental and control groups were selected purposively from the population of grade 11 MAN 1 Bandar Lampung, Indonesia in the academic year 2019–2020. A series of descriptive and inferential statistics were used to determine the effectiveness of the treatment on students' learning activities and critical thinking abilities. The results showed that the n-gain value of the experimental group ranging between 0.62 to 0.93 higher than the control group with n-gain ranging between 0.18 to 0.57. Furthermore, the analysis of the independent sample t-test yielded a sig < 0.05, which confirms the effectivity of molecular dynamics simulation in a discovery learning environment in fostering the critical thinking abilities. In addition, other findings also inform that discovery activities with computer simulations can increase student learning activities such as asking questions, communication attitudes, conscientiousness, and cooperation. Molecular dynamics simulation activities facilitate student learning and develop thinking skills, especially in discovering chemical concepts.**

***Index Terms*—Molecular dynamics simulation, discovery learning, molecular workbench, critical thinking skills, learning activities**

I. Introduction

Chemistry has the characteristics of abstract, complex materials, requiring laboratory activities and 3D space reasoning. It is not uncommon for students to think that chemistry is a difficult subject to learn at the high school and college level [1]. Some of the fundamental things that are the biggest challenges in learning chemistry are how to explain abstract concepts through multiple representations. Moreover, there are difficulties in connecting chemistry and everyday life phenomena, language barriers as well as chemical terminology [1–4]. This is because the special view of chemical phenomena is in many ways contrary to the intuitive and everyday views of students [1].

In science, especially chemistry, explaining an invisible phenomenon must be assisted by giving analogies, concrete models, or computer visualizations [1, 5]. Specific topics in chemistry that must use molecular representations include chemical reactions and changes, chemical bonds, chemical periodicity, acid/base chemistry, periodic table and trends, Lewis structures, molecular shapes, polarity, including chemical equilibrium [6–13]. Several studies confirm the use of visualization media and molecular representations and successfully improve cognitive skills [14–16], socio-cognitive interaction [17], virtual literacy [18–21], spatial ability [22–24], pedagogical understanding [25] and etc.

In general, molecular representations can be divided into statics (with a focus on symbolism and patterns) such as paper and pencil [9] or playdough-and-sticks [26] and dynamics (reactivity as process or as particles in motion) such as animation and simulation [27–30]. However, researchers tend to prefer dynamic over static representations in terms of increasing conceptual understanding [12, 31–33], mental models [27, 30], interest and motivation [34, 35], lower cognitive load [35], student learning and engagement [36]. Furthermore, Chang's research confirmed that learning using simulation leads to a significant improvement in student learning outcomes compared to only traditional laboratory practices [37].

Chemistry learning that involves dynamic representation can be done by integrating molecular dynamics simulation methods. Molecular dynamics simulation is a computational chemistry method based on classical mechanics which is able to simulate fluctuations in the relative position of a system of particles as a function of time [38]. With molecular simulations, the movement of all atoms and chemical reactions in detail can be observed at the atomistic level. Therefore, the integration of dynamics simulation in learning chemistry can effectively create enjoyable learning conditions and increase student engagement in learning [36].

Many studies on the implementation of molecular dynamics simulations in learning have been carried out using various computer simulation software. Some examples of recent research on this subject include those conducted by Schwedler and Kaldewey developed an online simulator called BIRC (Bridging Imagination and Representation in Chemistry) to support first-year students' physical chemistry learning such as ideal and real gases, energy distribution (entropy), changes in the concepts of internal energy, temperature, work, and heat [39]. Using a think-aloud protocol, interviews, and eight online questionnaires, they found that it created an interesting and enjoyable learning process, strengthened conceptual understanding, and encouraged a large number of students to volunteer to do some simulation exercises at home.

Another report submitted by Bruce also uses an online

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simulator called Virtual Substance [40, 41] and has succeeded in encouraging a better understanding of the origin of the macroscopic physical properties of gases. Application of this interesting application successfully leads students to learn the relationship between particle motion, macroscopic properties, and the mathematical laws of gases. Sevian *et al*. studied the impact of a context-based learning model with two different activities on chemistry students at two different universities [42]. It found that students who applied kinesthetic activity have stronger understanding while students who applied molecular dynamics have more sophisticated mechanistic reasoning and greater fluency of translation between contexts through increased use of chemist-specific language.

One of the molecular dynamics simulation-based software commonly used in learning chemistry is the molecular workbench. Molecular workbench was developed by the National Science Foundation and developed by Charles Xie in 2006. Molecular workbench is a software that can be used to learn about atomic and molecular science and can visualize atomic motion, waves, interactions of atoms based on equations and basic physical laws. In addition, molecular workbench can help teachers make it easier to teach abstract concepts with dynamic visualization without intimidating students with difficult mathematics [43]. Several studies report the use of molecular workbench applications for various purposes [43–48]. Khoshouie *et al*. proved that molecular workbench can help students gain a better understanding of chemistry on gas law, chemistry of molecular electronegativity, molecular and salt solutions [45]. In practice, simulation-based learning can be integrated into a learning environment with a constructivist philosophy such as discovery learning [49–52]. Specifically, Fermann *et al*. mention that the integration of molecular simulation in the discovery learning environment has a positive impact on increasing the level of critical thinking and scientific reasoning in general [52].

The integration of molecular simulation has many advantages and positive impacts on the learning of chemistry. Chemistry learning involves an understanding of abstract, complex concepts and spatial reasoning so that it requires the help of visualization and simulation tools to imagine chemical reactions at the molecular level. For example, in chemical equilibrium material, students will be asked to analyze and understand how molecules interact with each other in achieving equilibrium and shifting equilibrium in molecular view. Student learning activities with the help of molecular simulations in the discovery learning framework are believed to be able to improve students' critical thinking skills. This research aimed to investigate the effectivity of molecular workbench as a molecular dynamics tool in discovery-based learning environment to improve critical thinking skills in chemistry.

II. Research Methods

The sample of this study was 60 11th grade students at MAN 1 Bandar Lampung in the 2019–2020 academic year consisting of 30 students in each experimental and control class. The participants were chosen intentionally and were asked to join the study on a voluntary basis. Furthermore, a quasi-experimental with a matching-only pretest-posttest control group design [53] was used in this study and the duration of the study was four months from August to December 2019. The research procedure can be described as follows: preliminary stage, implementation, and end of the study. The preliminary stage consists of observations, learning models and research samples, and the preparation of simulations that will be used in learning. The research implementation phase completes the preparation of learning tools and a molecular workbench simulation that will be used. The implementation of discovery learning assisted by molecular dynamics simulation is guided by using the syllabus, lesson plan, and student's worksheet. The students' worksheet was constructed based on the stages of discovery learning, namely stimulation, problem statements, data collection, data processing, verification, and generalization. The validity of the content and construction of learning tools used in this study was based on the assessment of two experts, namely chemistry learning experts and computer-based learning experts. The Implementation of the treatments was done in five meetings including pretest and posttest.

Furthermore, the effectiveness of discovery learning assisted by molecular dynamics simulation was measured by critical thinking test instruments and students' activity observation sheets. Item questions on the test instrument were adapted from literatures [54–57] and validated by experts' judgments. It accommodated the five critical thinking skills [58, 59], i.e., observe, and judge observation reports (one question), deduce and judge deductions (two questions), make, and judge, inductive inferences and arguments (one question), and deal with things in an orderly manner (one question). The pre-treatment analysis included a normality and homogeneity tests of the average values. These tests were sequentially carried out using the Kolmogorov-Smirnov analysis method and the Levene test, while the similarity test for the two averages was carried out using the Mann-Whitney U non-parametric test with a significance level of 0.05. After that, the n-gain analysis [60], effect size with Cohen d, Glass's Δ, and Hedges's g, and the different analysis of the two n-gain mean values were carried out to obtain information on learning effectiveness. The test of the difference between the two means was carried out using a parametric statistical test with a significance level of 0.05. Data analysis of student participation in learning is done by comparing the number of activities and implementation of learning given by observers for each aspect of observation to the maximum score.

III. Result and Discussions

The effectiveness of the integration of molecular dynamics simulation technology in discovery learning was studied in this study to improve students' critical thinking skills and participation. The first stage was a pre-instruction analysis where an analysis was carried out to determine the existing conditions of the students' initial abilities. Respondent data were analyzed based on the average value of the pretest for further analysis of normality, homogeneity, and two-means equation test. The results showed that the average initial

ability of students was not normally distributed (sig. < 0.05) and homogeneous (sig. > 0.05). Furthermore, the analysis of students' initial abilities was carried out using a pretest instrument based on critical thinking skills. The results show that the average value of students' initial critical thinking abilities in the experimental and control classes is 8.41 and 7.89, respectively. The initial ability profile of the students in the two classes were then determined based on the similarity test of the two averages. Obtained the value of sig. (2-tailed) of 0.709 which indicated that the two classes initially had the same critical thinking ability.

The next stage was post-instruction analysis where at this stage the sample in the experimental class was treated by computer-assisted discovery learning, while the control class was taught by normal discovery learning. Respondent data at this stage was analyzed based on the comparison of the experimental and control class n-gain values on each critical thinking indicator. Furthermore, the value was analyzed for the difference between the two averages to measure the effectiveness of the treatment on critical thinking skills. The magnitude of the impact of molecular dynamics simulation was also studied by means of effect size analysis. The average n-gain values for the control and experimental classes were 0.44 and 0.79, respectively. In more detail, the comparison of the control and experimental class n-gain for each aspect of critical thinking skills is presented in Fig. 1.

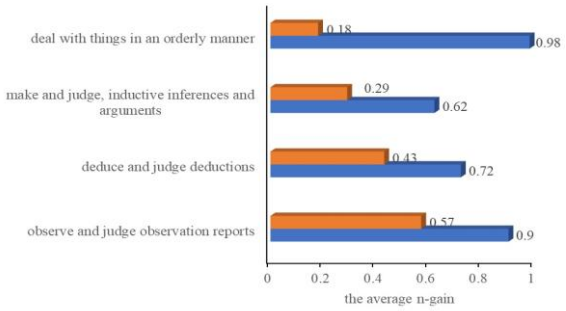


Fig. 1. N-gain of experimental (blue) and control (orange) group on the critical thinking abilities.

Critical thinking abilities [58] in this study were (a) observing, and evaluating observation reports, (b) concluding and evaluating deductions, (c) making, and evaluating inductive conclusions and arguments as three components of inference ability and (d) handling matters in an orderly manner as a non-constitutive but helpful ability that ideal critical thinkers possess. The following Fig. 2 is an example of a question on the ability to deduce and judge deductions:

Furthermore, normality and homogeneity analysis were carried out again on the n-gain value and obtained information that the post-instruction data were normally distributed and homogeneous. Furthermore, the two-average difference test was carried out using a parametric statistical test, namely the independent sample t-test. The results of the analysis produce a sig. value 0.000 (sig. < 0.05) which means that the integration of molecular dynamics simulation in discovery learning is more effective in improving critical thinking skills than discovery learning only. To see the magnitude of the effect, the effect size analysis was carried out by taking into account the Cohen d, Glass Δ, and Hedge g values as shown in Table I. Based on the three criteria the effect size in Table I, it can be identified that the integration of dynamics molecular simulation gives a large effect (d > 0.8) to the increase of students' critical thinking abilities.

Three students conducted an experiment on the effect of concentration on shifting equilibria. Firstly, they prepare a solution of iron (III) thiocyanate by mixing 5 ml of $FeCl_3$ 1M and KSCN 1M solution and pouring it into 25 ml of distilled water. The solution was then divided into four tubes. In each tube given treatment, namely:

a. Tube 1 as a comparison
b. Tube 2 added 3 drops of concentrated solution
c. Tube 3 added 3 drops of concentrated KSCN solution
d. Tube 4 added 3 drops of concentrated NaOH solution

Before the treatment was carried out on the four tubes, they first observed the color of the iron (III) thiocyanate solution. As the experiment progresses, they observe the changes that occur in each tube when given the treatment as above and compare it with tube 1.

Based on the experiment conducted by the student, answer the following questions (related to the experiment).

a. Make a table of observations based on the experimental illustration above!
b. What is the color of the iron (III) thiocyanate solution?
c. After each tube is given the above treatment, what changes occur in the iron (III) thiocyanate solution? and explain the changes that occur in the iron (III) thiocyanate solution after adding 3 drops each of concentrated $FeCl_3$ solution, concentrated KSCN, and concentrated NaOH!
d. Based on the observations made by these students, it turns out that the changes that occur in the iron (III) thiocyanate solution in tubes 2, 3, 4 are due to the addition of concentration. Explain what addition of concentration occurs in tubes 2, 3, and 4!

Fig. 2. Problems example of critical thinking abilities on indicator deduce and judge deductions adapted from Ghirardi *et al*. [54].

TABLE I: THE EFFECT SIZE ANALYSIS RESULT

Abilities	Experiment		Control		Cohen's d	Glass's Δ	Hedges's g
	Mean	SD	Mean	SD			
Observe and judge observation reports	99.67	1.77	60	48.19	1.16	0.82	1.16
Deduce and judge education	75	15.86	48.83	11.55	1.89	2.26	1.89
Make and judge inductive	65	21.63	36.67	12.27	1.61	2.31	1.61
Deal with thing	98.33	8.83	25.83	4.41	10.39	16.44	10.39

A. Students' Learning Participation in the Classroom

Student participation in learning and the implementation of learning were studied for three meetings to see whether or not there was an increase in student participation resulting from the treatment given. Students' participations observed in this study were questioning, communicating, observing thoroughly, and collaborating. The assessment of this participation is based on the observations of two observers of all students during the learning process using the observation sheet instrument. Examples of observation checklists on observation sheets include showing curiosity through observations during learning activities (questioning), being able to convey observations and expressing opinions during group discussions (communicating), showing a thorough attitude in observing experiments and molecular simulations (observing thoroughly), collaborate when doing experiments, groups, and solving problems (collaborating). The results of the observations are presented in Fig. 3.

From Fig. 3, student participation in class tends to increase from meeting 1 to meeting 3 for all aspects of class activities. For example, a 46.67% (14 students) asked questions at

meeting 1, an increase of 60% (18 students) at meeting 2, and more students who asked 80% (24 students) at meeting 3. Likewise, as with other activities that tend to increase from time to time. This is evidence that the integration of molecular dynamics simulation in discovery learning can increase student participation in learning. This is in line with the findings which confirms that computer aided learning has increased students' interaction, learning attitude, collaboration and motivation [61–64].

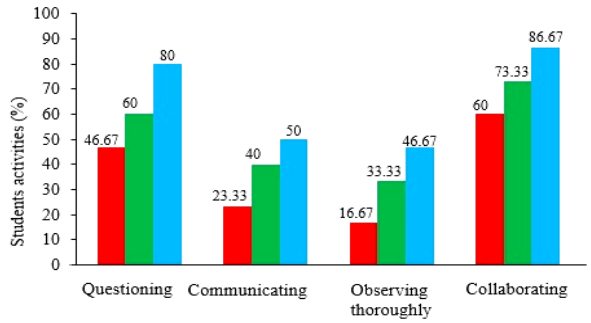


Fig. 3. Students' activities at the first (red), second (green), and third (blue) meetings.

B. Description of the Treatments on Three Meetings

1) At the first meeting

Students in the experimental class learned the effect of concentration changes on shifting equilibria (Le Chateliers' Principle). In the first stage: stimulation, teacher showed the phenomena in everyday life about the factors influencing the shifting equilibria. This is conducted to raise problems and foster students' curiosity and interest in solving problems. Then students were asked to identify the molecular representation of Iron (III) thiocyanate solution at the initial state and what happen with the system after the addition of $FeCl_3$, KSCN, and NaOH concentrations. In the next stage, students wrote down the problems found in the discourse. After finding problems, students learn to formulate questions. At this stage, the teacher can train how to formulate questions correctly based on the discourse.

Moreover, teacher trains students to make hypotheses in problem statement stage. The hypotheses will be used to assist the data collection process. At the data collection stage, students were asked to observe and identify the discourse given by the teacher to design the work steps in the laboratory experiment. Furthermore, students determined the variables, i.e., independent, dependent, and controlled variable, experimental procedures and materials. At this stage, students were trained to consider an appropriate procedure for laboratory experiment. Moreover, laboratory experiment with Iron (III) thiocyanate, $FeCl_3$, KSCN, and NaOH solutions was performed based on the procedures designed. All data were filled in the table of observations by the students after experiment. The implementability percentage at the first meeting was 57.60% as per observers' judgements. At this meeting, the students were unfamiliar with the discovery, so they felt it difficult to follow the learning mechanism. The less conducive classroom atmosphere also caused the unsuccessful implementation of the discovery learning model with molecular simulation at this meeting. The teacher also found it difficult when conveying the material.

2) At the second meeting

Data from the previous meeting was processed at this meeting (data processing stage). Students were asked to observe the reversible reaction of Iron (III) thiocyanate formation, and the color changes occurred. Students were asked to answer some questions related to experimental results such as chemical changes, reactions, shifting equilibria, concentrations effects, and action-reaction process corresponding to the Le Chatelier principle. Students were trained to state their interpretation related to the observation. At this meeting, students' ability in interpreting the experimental results was still not capable based on their answers.

Next stage was verification where the teacher asked students to carefully observe the animation of the concentration effects on equilibrium shifts and answer the questions in worksheet by referring the animations. The animations used in this stage can be seen in Fig. 4. Students observed the changes that occurred when the concentration of A molecules were increased or decreased. Critical thinking ability trained in this stage are the argumentation. Furthermore, students asked to generalize the concept (generalization stage) and then communicate the results to other students. At this stage, students were trained to draw conclusions from the observation results.

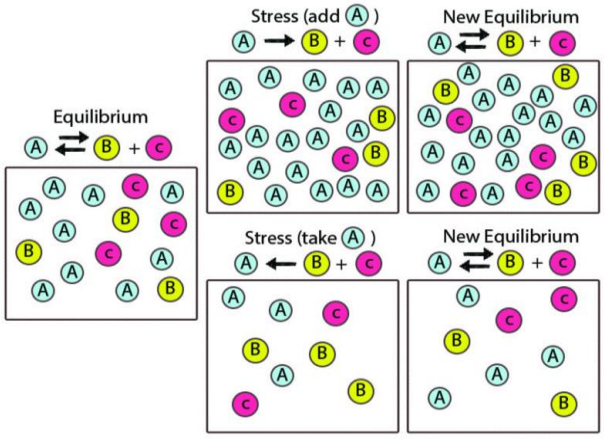


Fig. 4. Molecular workbench animation the concentration effect on the chemical equilibrium shifts.

The next lesson was the topic on the effects of temperature on the chemical equilibrium shift. At the stimulation stage, students were asked to observe the discourse and pictures on tube A containing NO_2 gases only at initial temperature (room temperature), tube B containing NO_2 gas with liquid nitrogen added (the temperature was lowered), and tube C containing NO_2 gases with heated water were added into the glass (temperature was increased). Students wrote down the problems found in the discourse. Then, students were asked to formulate questions after finding problems.

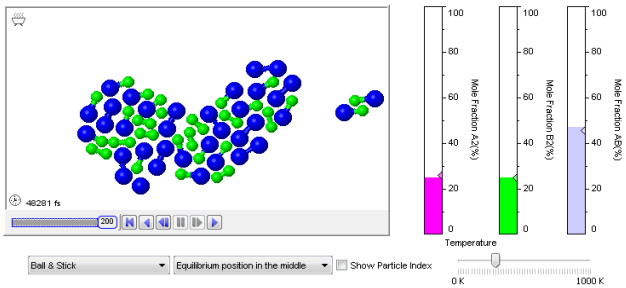
Students were asked to propose hypothesis based on the problems stated at the problem statement stage. Five students dared to propose their hypothesis. They were able to formulate the hypothesis correctly. Then, at the data collection stage, students were asked how to properly consider the experimental procedure. At this meeting,

students seemed able to consider the appropriate procedures, which is probably because they have been trained to determine and compare the related experimental procedures at the first meeting. At the second meeting, students were found getting used to the discovery learning with molecular simulation activities. The implementability percentage of the treatments at the second meeting was slightly higher (64.54%) than the first meeting as per observers' judgements.

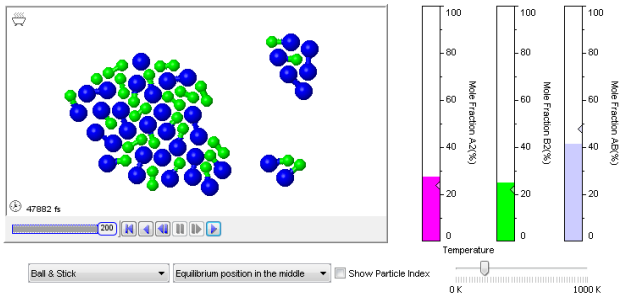
3) At the third meeting

The topic of the temperature effects on the chemical equilibrium shift was continued at the third meeting. At the data collection stage, students were asked to do experiments using copper (Cu) tape and concentrated HNO_3 solution. Students observed the reactions and recorded the observations in the table provided by teacher. Hereinafter, students were trained to state their interpretations correctly based on the facts at the data processing stage. Students were asked to write all the chemical reactions occurred in the experiment and answer the questions related to the topic. After that, students were asked to state their interpretation. At the verification stage, students were asked to observe the reaction between NO_2 and N_2O_4 gases and their observation results were compared with the information in data processing stage.

Furthermore, students observed the molecular simulation to understand the temperature effect on chemical equilibrium shift at the atomistic level. In the molecular workbench, there are several variables that can be changed such as temperature, molecular shape, state, and time. The application is also equipped with a menu bar containing file menus, edit, insert, view, options, bookmarks, collaboration, and help, where all the menu bars have their respective functions. Teacher also gave an introduction to the molecular simulation to prevent students' confusion. For example, the teacher said that the simulation provides the reaction between A2 and B2 gases to produce AB gases. Students were also asked to observe these reactions at initial temperature (300K), lowered temperature (250K), increased temperature (350K), and shifting of equilibria during the temperature changes as shown in Fig. 5.



(a)



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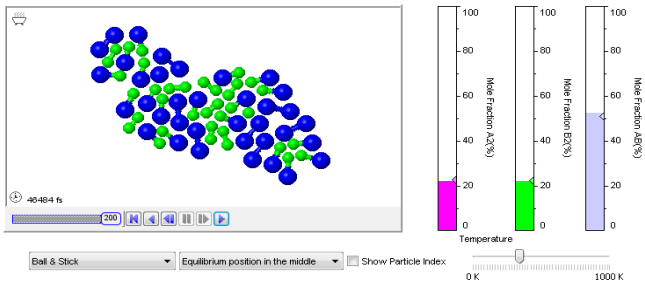

(c)

Fig. 5. Reactions at (a) initial temperature (300 K), (b) lowered temperature (250 K), and (c) increased temperature (350 K).

After simulation, students were asked to determine the number of molecules AB, A2, and B2 at initial temperature (300K), lowered temperature (250K), and increased temperature (350K). Moreover, students answered the questions related to the molecular simulations after filling in the observation table. In this case, students used their argumentation ability to solve the problems. At the generalization stage, students generated conclusions and met teachers' expectations. Then, the group representative conveys their works in front of the class. Observers found that the students were already familiar with the computer simulation-integrated discovery environments at the third meeting. Implementability percentage of the treatments at this meeting was the highest (74.61%). The interview results revealed molecular simulations is very helpful tools to represent and visualize the submicroscopic state of the molecules at the equilibrium positions and shifts. Moreover, students feel that using it is easier to find the concept of concentration and temperature effects on equilibrium shifts.

IV. Conclusion

This essay has discussed the impact of molecular dynamics simulation-integrated discovery learning environment on students' activities and critical thinking abilities. Normalized gain analysis proved that three critical thinking abilities and one non-consecutive but helpful ability, i.e., deal with things in an orderly manner, make and judge, inductive inferences and arguments, deduce and judge deduction, and observe and judge observation reports has significantly improved in the experimental group with n-gain value 0.98, 0.62, 0.72, and 0.90, respectively compared with control group with n-gain value 0.18, 0.29, 0.43 and 0.57, respectively. Moreover, Effect size analysis with the Cohen d, Glass Δ, and Hedge-g confirm that the integration of molecular simulation in discovery learning gave a large effect ($d > 0.8$) to the improve students' critical thinking abilities. Computer simulation activities have successfully helped students in learning the atomistic behavior of equilibrium reactions and shifts in equilibrium positions caused by concentration and temperature changes. The findings of this research provide insights for the effectivity of the discovery learning assisted with molecular dynamics simulation. Learning chemistry using computer simulation in a discovery learning environment is very recommended to motivate students to actively participate in learning. This study also suggests to be

implemented on other topics of chemistry such as stoichiometry, atomic structure, acids and bases, chemical reaction kinetics that require submicroscopic representations especially in molecular dynamics simulation.

CONFLICT OF INTEREST

The authors declare no conflict of interest

AUTHOR CONTRIBUTIONS

Andrian Saputra and Lisa Tania conducted the research, analyzed the data, and discussed the results. Ila Rosilawati discussed the results and approved the final version.

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