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Incorporate Computational Chemistry as an Alternative for Chemistry Laboratory Work at High School Level

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Abstract

Carrying out chemistry laboratory activities at high school level in Indonesia is a challenging task. Lack of equipment, chemicals, cost, and even worst no laboratory infrastructuresforce wet laboratory practicehardly exist in mosthigh schoolsin this country, especially at Lombok Island, West Nusa Tenggara province. This pilot project focused on incorporate computational chemistry as an alternative for chemistry laboratory work at high school level. It describes the effectiveness of computational chemistry software for replacing wet laboratorypractice. We have studied what topics are essential and what topics are student struggled with, chosen computational chemistry software and conducted teacher motivation survey. This project is promising and has a strong impact in the future but improving the current high school technology is a necessity.

Keywords: *computational chemistry, high school, laboratory*.

1. Introduction

Chemistry lab is one of the core activities on chemistry learning included in the level of high school. However, the implementation of the chemistry lab faced many obstacles in Indonesia (Coppola, 2008). The high workload of teachers lead to less motivated to plan, prepare and conduct the chemistry lab. The other obstacles are the expensive cost of laboratory practice, time consuming, limited equipment and chemicals (Jansen-van Vuuren, 2013) as well as the possible dangers during chemistry practicum. In addition, many high schoolsin Indonesia do not have a chemical laboratory infrastructure, no laboratory building and waste treatment plan. It makes chemistry practicum did not go well so that chemistry learning process does not produce the optimum result.

Chemistry is a science-based theory and experiment. Theory without chemistry laboratory practice leads to the students miss understanding of the chemistry key concepts. Many chemistry topics are abstract in concepts so that it is considered difficult. Absorbing these abstract topics within a relatively limited time with no chemistry laboratory practicum makes many students fail in chemistry class.In addition, the learning process emphasizes only on the theory without practical would be boring and less attracting.

Applying computational chemistry as an alternative chemistry lab is a solution for this problem. Computational chemistry methods are very flexible. All topics on the chemistry lab ranging from simple level to level difficult can be easily modeled using computational chemistry. The availability of a wide range of computational chemistry software for free can be used by teachers as a substitute for chemistry lab at the school (Fortenberry, 2015). The other advantages of using computational chemistry as an alternative for practicum in high schools is low cost, highly accuracy, less time consumption, harmless and certainly help improve students'

understanding of chemical topics (Sendlinger and Metz, 2010; Ochterski, 2014).

2. Materials and Methods

The aims of this project are to determine the most suitable software for lab-based computational chemistry in high school. Secondly, to determine the essential chemistry topics for computational chemistry based practicum. Thirdly, to study the teacher motivation to implementlab work in chemistry learning process. Based on the above objectives, the methodology of this project are a survey of chemistry topics, software review, and implementing a lesson plan.This pilot project was sampling two high schools: SMAN 1 Narmada and SMAN 2 Narmada atLombok Island, West Nusa Tenggara province, Indonesia.

3. Results and Discussion

3.1. Program Review.

Some programs were reviewed as a prime candidate to be used as alternative for replacing the lab work in high school. The program can be seen in Table 1. The program selected based on ease of installation, ease of use, and compatibility with chemical topics.

Table 1. Potential Program Fitures

No	Program	Web based	Easy to Install	Easy to Use 1= very difficult 5 = very Easy	Finalist
1	NWChem*[1]	No	No	2	No
2	Hyperchem[2]	No	Yes	4	Yes
3	Gaussian[3]	No	Yes	2	No
4	Chemlab[4]	No	Yes	5	Yes
5	WebMo[5]	Yes	No	4	No
6	ACD/ChemSketch[6]	No	Yes	5	No

*1. Valiev, 2010; 2.Froimowitz, 1993; 3.Frisch, 2004; 4.Maciejowska, 2009; 5.Schmidt, 2007; 6.Spessard, 1998.

Two programs were chosen because they fit the categories: Hyperchem and Chemlab. Both programs were chosen due to they do not need the internet, and can be installed locally. This is advantageous because of limited access to the Internet at school. Hyperchemwas chosen because it could represent aspects of chemistry laboratory microscopically, easy installation, windows-based so it can be easily used by teachers. In addition, the facilities of Hyperchem calculations are fairly complete. The calculation can be performed at the various levels ofcalculations: molecular mechanics, semi-empiric, *abinito*, density functional theory and post-*ab initio*.ChemLab was chosen due to it can represent the macroscopic aspects to bridge the wet laboratory practice. This program is also easy to use, easy to install and has the complete featuresfor virtual practicum.

Some programs were eliminated due to a major flaw in installation, or difficult to use so they were not suitable for this project. Although Nwchem and Gaussian relatively easy to install and havecomplete features, very complicated in the operation so that NWChem and Gaussian wereeliminated. Although easy to install and use, ACD/ChemSketch only for visualization and cannot be used for calculating chemical system so thatit was eliminated.

3.2. Chemistry Essential Topics

In order to obtain topics that are essential for chemical lab-based computing, the survey carried out on teachers. The survey results showed some of the main topics that need to be applied as the main topic chemistry lab work. Teachers suggest topics: atomstructures, periodic properties of the elements, acids and bases, physical and chemical properties of substances, molecular geometry, energy and thermodynamics and organic chemistry to be involved in the lab.

Once the essential topic is decided then the next step is to develop a practicum in accordance with software that has been previously based on these topics. It is found that topics such as the atomic structure, the periodic properties, molecular geometry, energy and thermodynamics and organic chemistry lab are suitable to be performed using Hyperchem. In contrast, topics such as acid-base and the physical and chemical properties of substances can easily do with ChemLab.

3.3. Teacher Motivation

The survey was also used to measure the level of motivation of teachers in implementing chemical lab. A total of 20 teachers were taken as a sample to determine the chemical lab work implementation and motivation before and after the introduction of computational chemistry technologies for chemical lab. The survey showed that nearly 85 % of teachers in Lombok Island did not carry out routine chemical lab. In contrast, survey showed that the motivation of teachers in conducting chemistry lab was categorized high (motivation score = 3.1 of interval 1-4). This contradiction may due to many obstacles as mentioned previously.

The introduction of computational chemistry as an alternative chemistry lab did not change the level of motivation of teachers for implementing chemistry lab in learning. The good news is our observation showed that the teachers at partner schoolshave started to carry out routine chemical lab. We believe soon it will be followed by other school in West Lombok district.

4. Conclusion

Chemistry lab-based computational chemistry can be an alternative solution for the chemistry lab at the high school. Practical chemistry-based computing has advantages such as efficiency of time, effort, and cost, minimize the hazards and waste practicum. Teachers have high motivation to carry out practical activities after the introduction of computational chemistry. Chemistry lab-based computing is very useful for teachers and students to optimize the learning process, especially in high school.

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