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e-Chemify: A 2D Simulator Virtual Laboratory for Chemical Experiments

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Abstract

E-Learning is described as a mode of acquiring knowledge through the use of modern technologies to access educational resources outside the traditional classroom set up. With these concepts, the proponents decided to develop this project to utilize computer in aiding in learning particularly Chemistry Laboratory. In a survey conducted to Mapua SHS students and Chemistry Professors, most agrees that a chemistry laboratory simulation would help them in the subject. The project aims to help students understand and prepare them for the actual laboratory experiment because students lack preparation for the experiment and the familiarization of equipment, utensils and procedures for that experiment. The simulation of laboratory experiments will focus on trying to recreate the outcome of the real experiment in a simulated environment while also having real-life visual and audio for the students. Tools for developing simulation applications have evolved from simulation subroutines to high level process languages built to visual development. A feature of a computer-based simulation is the possibility to replicate every possible scenario at a very low cost.

Keywords
E-Learning; Simulation; Laboratory Experiments; Simulated Environment

1. Introduction
Nowadays, computers are beneficial in modern education like laboratory being used for interactive lectures, online quizzes, animations, collaborative learning tool to aid in accelerating data collection, analysis and especially pre-laboratory tutorials (Loveys and Riggs 2019). An example of this is the CISCO packet tracer (Alfarsi et al. 2019). Experimental simulation offers an effective solution for peers in the science to meet their laboratory requirement.

Technology having the ability to bridge gap in traditional learning is often the pivot of debate than its value to boost learning (Abu Talib et al. 2021). Studies have shown that the utilization of computer simulations for learning supplements for subjects (Novaliendry et al. 2020) like biology, geology, physics, math and chemistry does promote learning (Zargaran et al. 2020). Simulated Activities have its edge over hands-on laboratory work such as enabling students to do more hazardous and complicated experiments (Mahtari et al. 2020) without risking the student or the environment, they can also obtain accurate results more quickly without factors that increase the percentage errors such as air friction, pressure, room temperature, impure or contaminated chemicals, faulty apparatus and inaccurate weighing scale (MaKechnie et al. 2020). Disadvantages includes the lack of the capability to experience the actual feel of the experiment and errors associated with laboratory simulations (Ratcliffe et al. 2021). Available software for simulations in chemistry varies depending on the graphics available (Haydary 2019). The simulation of laboratory experiments will focus on trying to recreate the outcome of the real experiment in a simulated environment while also having real-life visual and audio for the students (Hamilton et al. 2021). By engaging students in making a strong impression that will stimulate more senses with the expectation that the information will be more understandable strategy. This study designed a wide range of learning aids in a chemistry course to students by providing an equal amount of encounter in standard laboratory practice using a simulated environment.

1.1 Objectives
The project is about a 2D simulator of a virtual laboratory for chemical experiments in mobile application. The project developed a mobile application that will simulate, monitor, and assess the process of Chemistry laboratory experiments as learning-aid for students. Specifically, the project aims to simulate the process of Chemical laboratory experiments in the form of multimedia by animation, to monitor the student users that will simulate the laboratory experiments by enrolling to a class created by an instructor, and to assess the student's performance based on their answers to the exercise questions and on the results of the simulation performed.

1.2 Scope of the Study
Simulations are often used as preparation for laboratory work by enhancing learning and performance by providing students with basic concepts and principles prior to the actual laboratory work. The developed mobile application would be of help for the Senior High School student of Mapua Makati in studying and practicing their Chemical Laboratory Experiments and provide service improvement for the system as needed.
The developed application run on Android OS latest version; it has animation, sounds, and effects. The application consists of a Login Module, Register Module, Class Module, Assessment Module, Process Module, Workspace Module, and Tutorial Module.

2. Literature Review
Teaching and adapting more theoretical subjects, such as computer systems, where more elevated amount of student's creative ability is important to comprehend propelled topics can be emphatically upheld through a technique called visual learning (Vieira et al. 2018). Students can more effectively comprehend and adapt the data from the subject, when they can outwardly perceive how it truly functions (Williamson et al. 2020). Instructors can teach the subject using simulation tools and practical examples, instead of simply discussing hypothetical facts. This paper introduces the highlights of a visual learning apparatus, a computer network simulator technology, which is accessible for all students taking Chemical laboratory classes for General Chemistry.

2.1 Simulation Technology
Simulation Technology is a wide collection of methods used to ponder and examine the behavior and execution of actual or hypothetical frameworks (Mulyadi et al 2021). Studies about simulation are performed, not on this present reality framework, but rather on an (ordinary computer-based) model of the framework made to study certain framework elements and characteristics. Simulation is both an experiment and a workmanship (Li et al. 2021) or art in the development of the precise, "substantial" model that catches the fundamental components of the framework, and the utilization of the model to analyze framework behavior under different situations.

Chemistry involves experimenting, compound building and specializes in innovation (Hoffman and Gastreich 2019). With the advanced society, the simulation technology continues to develop, and the present-day factories have highly increased its level of mechanization. At work, the factory operators cannot directly observe the production process due to the factories are irregular and at the same time operators can't comprehend the procedure of driving and parking when working in the factory. Furthermore, irreproducible factors such as the operator's lack of precise judgement during the process of actual fault point and the ability to rapidly solve the issues, and to tackle these issues, the computer simulation has been generally utilized in chemical industries (Pan 2019). Computer intelligent simulation for laboratory experiments utilizes computer to make a virtual chemical laboratory operating environment, including virtual experimental apparatus such as beaker, flask, hob, mixer, and other devices and so on, that the system will operate to make the experiments (Ali and Ullah 2020).

As shown on Figure 1, in preparation for the laboratory, a chemical experiment starts with obtaining the experiment principles and its objectives. Experiment principles serves as the laboratory guideline where they obtain the step-by-step operation process and the list of experiment instruments to be used. Experiment objective sets the learning goals that are linked to achievement and is dependent on context, this will lead to better understanding about efficacy of the laboratory curriculum, this gives the effective data and information for the experiment and every operation function.

The purpose of chemical laboratory experiment is to teach students and cultivate them into a high-quality chemical expert, with a specific end goal to accomplish the objectives of developing talent, for the laboratory management to be improved. Using a programmed simulation and intelligent control, it can lessen the repetitive process in the chemical experiment, be more knowledgeable with the basic unit of chemical operation method, and to have deeper

understanding of the changes of every parameter and experimental principle. Chemical combination or reaction simulation can help specialists to enhance the capacity of finding errors in the process and the capabilities to solve the issue in time.

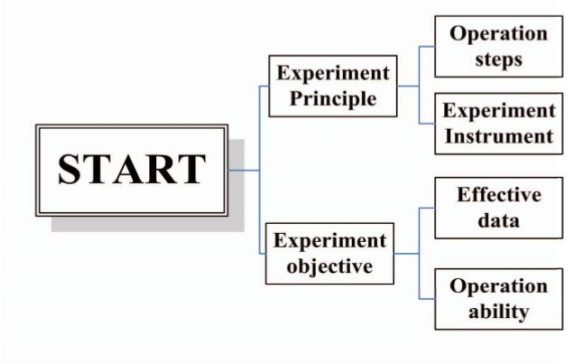

Figure 1. Software block diagram of a chemical experiment computer simulation

2.2 Mobile Application Development

Developing applications for mobile phones requires thinking about the imperatives and highlights of the devices. Mobile phones keep running on battery and have weaker processors than personal computers and more features such as location and cameras (Pramanik et al 2019). Developers must consider about many screen sizes, hardware specifications and configurations because of extreme competition in mobile software.

Development of mobile applications requires utilization of specific integrated development environments. Mobile applications are tested inside the development environment utilizing emulators and later subjected to handle testing. Emulators give a reasonable method to test applications on mobile devices to which developers might not have physical access (Wang et al. 2021). As a major aspect of development process, mobile user interface design (UI) is likewise an essential in the production of mobile applications. Mobile user interface considers imperatives and contexts, screen, input, and mobility as outlines.

2.3 Android Operating Systems

A mobile's operating system (OS) in view of the Linux and is currently being developed by Google. With a UI based on direct control, Android is outlined essentially for touchscreen devices such as smartphones and tablet PCs, with UIs for TVs (Android TV), cars (Android Auto), and wrist watch (Android Wear). The operating system utilizes touch inputs that freely relate to real-world actions, such as swiping, tapping, squeezing, and reverse squeezing to control on-screen objects, and a virtual console (Mahmood et al. 2019).

2.4 Firebase

A mobile platform that helps users rapidly develop astounding applications, develop user base, and acquire more cash (Lashitew et al. 2019). Firebase is comprised of complementary features that users can mix and match to meet their requirements, with Google Analytics for Firebase at the center. Users can explore and integrate Firebase services in their application directly from Android Studio utilizing the Assistant window shown in the figure below. For enhancing application quality, Firebase provides the user insights into application performance and stability, so the user can channel their resources effectively (Khawas and Shah 2018).

3. Methods

E-Chemify: Virtual Laboratory for Chemical Experiments 2D Simulator - Android Application is developed in Unity game engine for the developers to build the system's parts rapidly since Unity has quick prototyping capacities. The language used for scripting in Unity is C# for the developers to completely code the system with precise control.

The system also adopted Computer Intelligent Simulation Technology in the Application of Chemical Experiment by having the chemical laboratory environment, laboratory apparatuses, and the chemicals virtualized. Regarding the Experiment principles and Experiment objectives, the system has step by step process, and stated objectives for every

laboratory experiment. Like Cisco Packet Tracer, E-Chemify have a drag and drop functionality for the user to easily manipulate the laboratory equipment and chemicals on the workspace.

3.1 Planning and Design

The content of the developed system is based on Senior High School's Chemistry Laboratory Manual Part 1. The laboratory apparatuses were also stated from the laboratory manual. The laboratory manual contains five experiments and each experiment has the following parts: Introduction, Objectives, Materials, List of Apparatus, Safety Precaution, Procedure, Waste Disposal, References, and Report Form. The proposed system will be tested and evaluated by three (3) Chemistry Professors.

The developed system used Unity Software tool and C# in developing the virtual laboratory mobile application and Firebase for the system's local database. The target users for this project are the Senior High School students of Mapua University that are taking or will take General Chemistry 1. The Preferred Server, Hardware and Software Specifications are as follows: Android Phone with OS version 8.0 up to latest version with 2GB of free disk space and 2GB of RAM.

The application run easily on the machine and shall not breach privacy. As a functional requirement, the developed system have a user login, registration interface, assessment view functionality which will display the student's activities and scores, student roster, gradebook, and exercises, a process view functionality which will display the platform where the user simulates chemical process, workspace view functionality which will display the platform where the user simulates chemical process, tutorial view functionality which will display the procedures for each laboratory activity, and loading screen/s that will load the resources in the background.

4. Analysis and Design

The developers analyzed first the requirements to obtain the proper business logic, and afterwards present a functional database and infrastructure design that will fulfill the scope and requirements based on the analysis. Use case, early design concepts and outputs, scenarios, entity relationship diagram, data dictionary, and user matrix are included for detailed explanation of business logic of the system in this chapter. This project is composed of seven modules as follows:

Login Module. This module contains accounts credentials such as username and passwords as shown in Figure 2.

Figure 2. Screen Mockup for Login Page

Register Module. Allow users to register and choose account type as shown in Figure 3. The accounts can be either a student or instructor account with different privileges over the application. The Instructor Account is allowed an access to the application, workspace, tutorials, gradebook, editing and grading of student's submitted exercises, and generate class keys. The Student Account must enter class key to enroll and is allowed an access to the application, workspace, tutorials, and gradebook, but is not allowed an access to edit an exercise, grading of exercises, and view exercises of students.

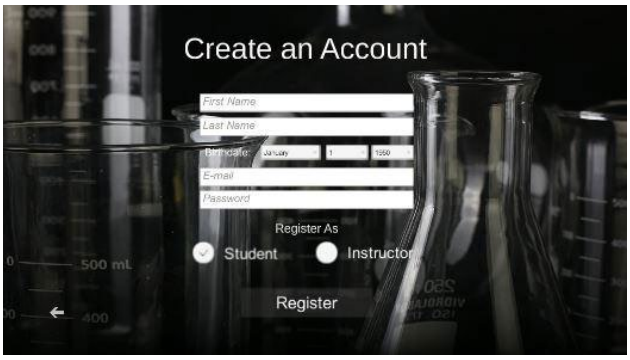

Figure 3. Screen Mockup for Registration Page

Class Module. This module generates class keys which contains 10 characters with integer and letters (i.e. ABC456789D). Each class key will have one instructor and many students as shown in Figure 4.

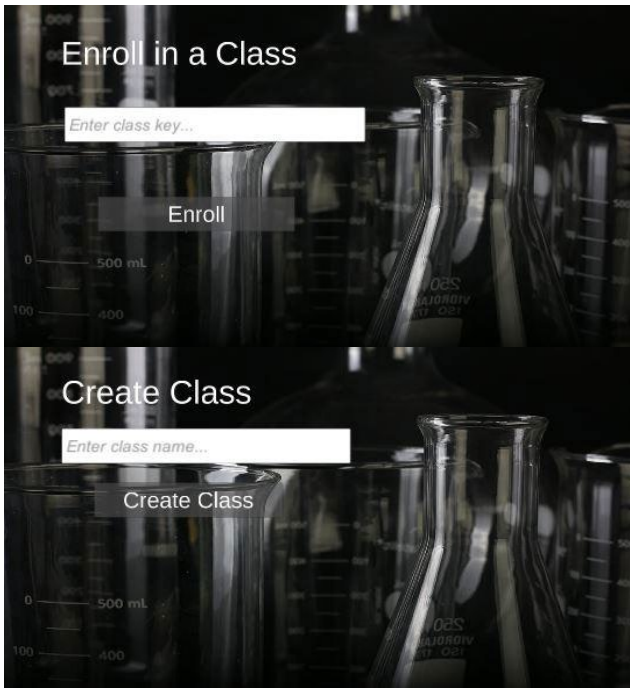

Figure 4. Instructor User's Class Key Generator Page

Assessment Module. This module will provide the gradebook which will display the recorded scores from each exercise, the premade exercises, experiment procedures, and report forms as shown in Figure 5. Instructors can also modify the number of attempts; it can be set to 'unlimited' attempts. If not set, it will be set to default with a minimum value of 1 and maximum value of 5. Instructors are also allowed to modify Time limit; the value can be set into minutes with a minimum value of 60 minutes and maximum value of 120 minutes. If not set, the default is 'no time limit'.

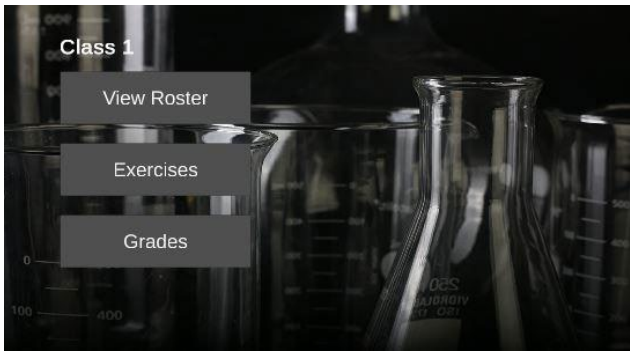

Figure 5. Screen Mockup for Assessment Module

Process Module. This module contains processes for combining elements into compound elements, for combining substance and equipment, and combining substance and substance as shown in Figure 6.

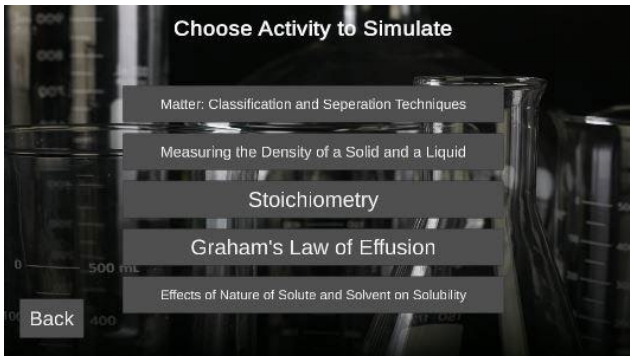

Figure 6. Screen Mockup for Laboratory Activity options

Workspace Module. This module provides the space where the user will work on. It will contain the Element Menu where they can access the elements, and the Equipment Menu where they can access the equipment as shown in Figure 7. A Tutorial Module contains the procedures for each laboratory experiments. Functionalities includes those users can select apparatus, select chemicals, drag-and-drop, view procedures, display real-time workspace, and view assessment module.

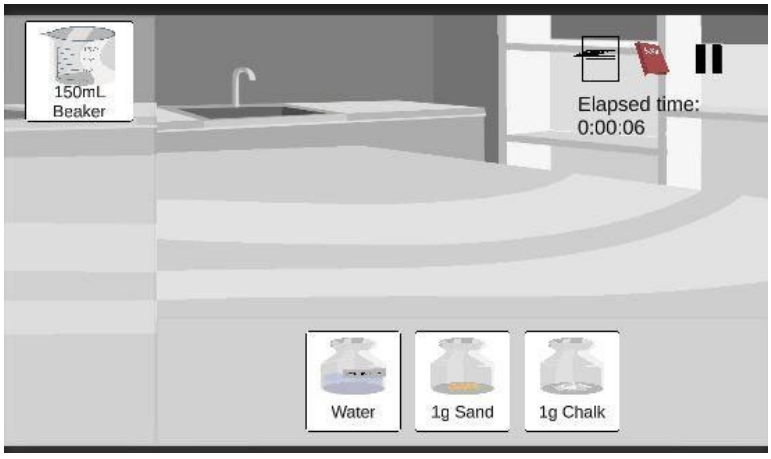

Figure 7. Screen Mockup for Workspace Module

The system architecture for E-Chemify is shown in Figure 8. The user interface will be designed according to Graphics, Sounds, and Touch by utilizing an engine where the application will run. program interfaces including: Assets for handling resources such as sounds, sprite, and scripts; Physics 2D for handling the physics of the objects; Audio, which is usually integrated with assets, for managing which assets would be the source and the listener of the audio; and the Multi touch input/Touch Input for handling user touch input.

For the data storage, fixed assets such as equipment and substances would be stored in a local database using SQLite. On the other hand, user accounts and class related data would be stored in a cloud using Firebase SDK for Unity. Firebase would be utilized for its real-time database, cloud storage and cloud messaging.

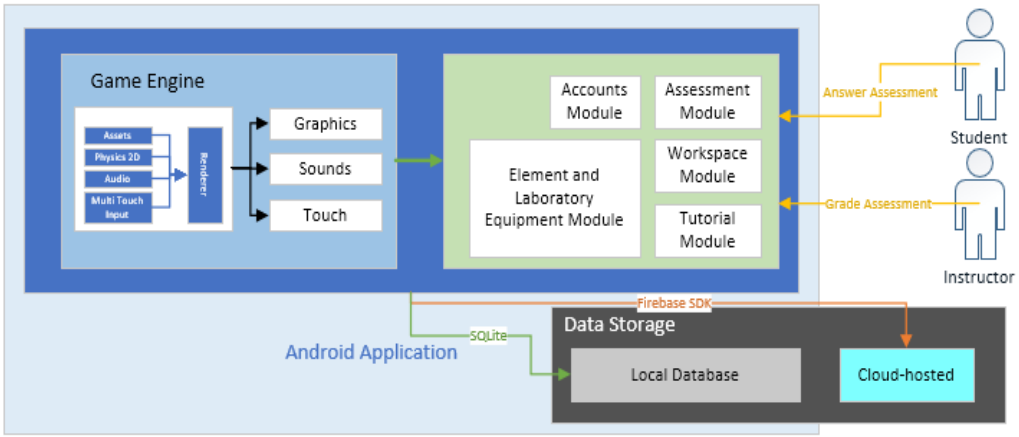

Figure 8. System Architecture of E-Chemify

The network architecture of the developed system is shown in Figure 9. Data with regards to accounts and class module will be stored in a real time database that comes from Firebase SDK. These data are in JSON format and would be synced between users in real time. The Firebase SDK will also have a local cache to store changes in case the user disconnects from the internet and the moment the user reconnects, the changes made would be synced automatically.

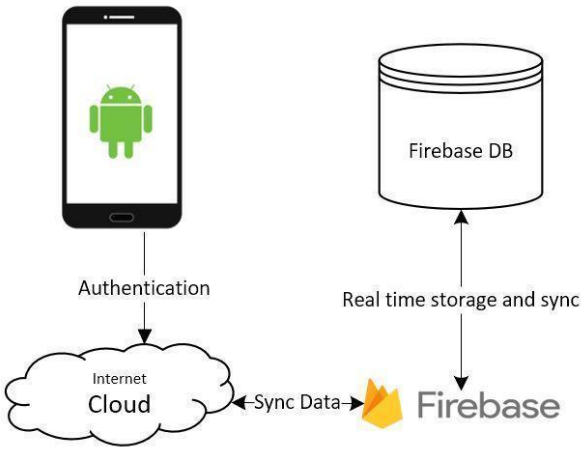

Figure 9. Network Architecture for E-Chemify

5. Implementation and Testing

The developers code and created prototypes of the system, animations, and other assets that would be used for the system using different tools for development. System development is performed in a game engine and involves adding of application program interfaces for the database and other features of the software. Additional resources, features, and changes for the system during iteration process are also done in this phase. The developers generate test results from the tests performed on the system to resolve probable bugs, errors, and performance issues of the software.

The result of user acceptance testing (UAT) from students is shown in Table 1, Table 2 and Table 3. There were seventeen (17) respondents on the UAT. For graphical user interface design (GUI), the result shows on Table 1 that the respondents are satisfied with the developed systems GUI. The result of functionality testing, as shown in Table 2, presents that the students agree that the system functions well as intended.

Table 1. GUI Design UAT Results from Students

Criteria	Excellent	Very Good	Good	Fair	Poor
1. Text is readable/easy to understand	9	8			
2. Smooth navigation	12	2	3		
3. Buttons are functioning properly and easy to identify	11	5	1		
4. Color scheme and design are pleasing to the eyes and consistent	3	12	2		
5. Color scheme is consistent throughout the whole system	7	8	2		

Table 2. Functionality UAT Results from Students

Criteria	Yes	No
1. User requirements are met.	16	1
2. Only authorized credentials are accepted by the system.	15	2
3. The system can view each module.	15	2
4. The system can choose which experiment to simulate.	15	2
5. The system should allow the user to register their credentials.	14	3
6. The system should allow the user to create a class by generating a class key.	15	2
7. The instructor can add premade lab experiments to a class.	15	2
8. The system should allow the user to add instructions to an added premade experiment	16	1

The result of UAT of students for accuracy of the input and output of the developed system shown in Table 3 illustrates that respondents were able to easily understand the lesson and its all correct.

Table 3. Accuracy UAT Results from Students

Criteria	Yes	No	Comments
1. The system's virtual representation of laboratory assets is accurate.	15	2	
2. The database is up to date and correctly synced.	15	2	
3. The information displayed on the system are correct.	15	2	
4. Account settings and credentials are correct and synced on the database.	15	2	

The same questionnaire for UAT was given to Chemistry instructors and all resulted to satisfactory result.

6. Conclusion

The use of E-Learning is improving the way the teachers interact with their students and enhance the distribution of educational content than the traditional classroom. The problem of chemistry students is that they lack preparation for the upcoming activity. By using the E-Learning application, the students can practice for their activity. Therefore, the use of E-Learning is beneficial to this modern age where evolving technologies can help bridge the gap between technology and learning.

The system, named E-CHEMIFY: A Virtual Laboratory for Chemical Experiments 2D Simulator – Android Application will help the students familiarize with the right equipment to use for the experiment and be mentally prepared for the activity. The system can simulate chemical process of each laboratory activities from the Senior High School's General Chemistry 1 Manual and an instructor can assess a student enrolled in their class. It also includes various features such as Class Key Generator, Student Roster, Gradebook, and Edit Exercise.

References

Loveys, B.R. and Riggs, K.M., Flipping the laboratory: improving student engagement and learning outcomes in second year science courses. *International Journal of Science Education*, 41(1), pp.64-79, 2019.

Alfarsi, G., Jabbar, J., Tawafak, R.M., Malik, S.I., Alsidiri, A. and Alsinani, M., Using Cisco Packet Tracer to simulate smart home. International Journal of Engineering Research & Technology (IJERT), 8(12), pp.670-674, 2019.

Abu Talib, M., Bettayeb, A.M. and Omer, R.I., Analytical study on the impact of technology in higher education during the age of COVID-19: Systematic literature review. *Education and information technologies*, 26(6), pp.6719-6746, 2021.

Zargaran, A., Turki, M.A., Bhaskar, J., Spiers, H.V.M. and Zargaran, D., The role of technology in anatomy teaching: striking the right balance. *Advances in Medical Education and Practice*, 11, p.259, 2020.

Novaliendry, D., Darmi, R., Hendriyani, Y., Nor, M. and Azman, A., Smart learning media based on android technology. *International Journal of Innovation, Creativity and Change*, 12(11), pp.715-735, 2020.

Mahtari, S., Wati, M., Hartini, S., Misbah, M. and Dewantara, D., The effectiveness of the student worksheet with PhET simulation used scaffolding question prompt. *In Journal of Physics: Conference Series* (Vol. 1422, No. 1, p. 012010). IOP Publishing, 2020.

McKechnie, T., Levin, M., Zhou, K., Freedman, B., Palter, V.N. and Grantcharov, T.P., Virtual surgical training during COVID-19: operating room simulation platforms accessible from home. *Annals of surgery*, 272(2), p.e153, 2020.

Ratcliffe, J., Soave, F., Bryan-Kinns, N., Tokarchuk, L. and Farkhatdinov, I., Extended Reality (XR) remote research: a survey of drawbacks and opportunities. *In Proceedings of the 2021 CHI Conference on Human Factors in Computing Systems* (pp. 1-13), 2021.

Haydary, J., Chemical process design and simulation: Aspen Plus and Aspen Hysys applications. John Wiley & Sons, 2019.

Hamilton, D., McKechnie, J., Edgerton, E. and Wilson, C., Immersive virtual reality as a pedagogical tool in education: a systematic literature review of quantitative learning outcomes and experimental design. Journal of Computers in Education, 8(1), pp.1-32, 2021.

Vieira, C., Parsons, P. and Byrd, V., Visual learning analytics of educational data: A systematic literature review and research agenda. *Computers & Education*, 122, pp.119-135, 2018.

Williamson, B., Bayne, S. and Shay, S., The datafication of teaching in Higher Education: critical issues and perspectives. *Teaching in Higher Education*, 25(4), pp.351-365, 2020.

Mulyadi, M., Tonapa, S.I., Rompas, S.S.J., Wang, R.H. and Lee, B.O., Effects of simulation technology-based learning on nursing students' learning outcomes: a systematic review and meta-analysis of experimental studies. *Nurse Education Today*, 107, p.105127, 2021.

Li, Z., Cao, Y. and Luo, J., Application of virtual simulation technology in chemistry teaching. *In E3S Web of Conferences* (Vol. 267, p. 02067). EDP Sciences, 2021.

Hoffmann, T. and Gastreich, M., The next level in chemical space navigation: going far beyond enumerable compound libraries. *Drug discovery today*, 24(5), pp.1148-1156, 2019.

Pan, J.Y., Engineering chemistry innovation. *ACS Medicinal Chemistry Letters*, 10(5), pp.703-707, 2019.

Ali, N. and Ullah, S., Review to analyze and compare virtual chemistry laboratories for their use in education. *Journal of Chemical Education*, 97(10), pp.3563-3574, 2020.

Pramanik, P.K.D., Sinhababu, N., Mukherjee, B., Padmanaban, S., Maity, A., Upadhyaya, B.K., Holm-Nielsen, J.B. and Choudhury, P., Power consumption analysis, measurement, management, and issues: A state-of-the-art review of smartphone battery and energy usage. *IEEE Access*, 7, pp.182113-182172, 2019.

Wang, W., Lam, W. and Xie, T., An infrastructure approach to improving effectiveness of Android UI testing tools. *In Proceedings of the 30th ACM SIGSOFT International Symposium on Software Testing and Analysis* (pp. 165-176), 2021.

Mahmood, Z., Bibi, N., Usman, M., Khan, U. and Muhammad, N., Mobile cloud based-framework for sports applications. *Multidimensional Systems and Signal Processing*, 30(4), pp.1991-2019, 2019.

Lashitew, A.A., van Tulder, R. and Liasse, Y., Mobile phones for financial inclusion: What explains the diffusion of mobile money innovations? *Research Policy*, 48(5), pp.1201-1215, 2019.

Khawas, C. and Shah, P., Application of firebase in android app development-a study. *International Journal of Computer Applications*, 179(46), pp.49-53, 2018.