The formation of an icosahedral structure with simulation of hydrogen adsorption on silica gel

A Muliawan¹, A Yani² and F Amalinda³

¹ Physics Laboratory, Dept. of Electrical Engineering, Sekolah Tinggi Teknologi Bontang, 75313, East Kalimantan, Indonesia
² Dept. of Mechanical Engineering, Sekolah Tinggi Industri Bontang, 75325, East Kalimantan, Indonesia
³ Faculty of Public Health, Universitas Muhammadiyah Palu, 94118, Central Sulawesi, Indonesia

Email: ariefstitek@gmail.com

Abstract. Hydrogen is one of the energy of the future that continues to be carried out research because it is environmentally friendly. Hydrogen distribution and storage processes that require large costs. Silica gel is a solid chemical that is widely used as an adsorbent. This research aims to study the Icosahedral Structure of hydrogen adsorption on silica gel. Experimental research is constrained by costs, so it needs to be supported by other methods such as molecular dynamics simulations. The results of the study show that increasing the temperature and pore size will reduce the amount of hydrogen absorbed.

1. Introduction
Hydrogen is very promising as a fuel for the future. Problems that arise are still related to the way they are stored until now. The main problem related to hydrogen is leakage in the tank during storage, maintenance and safety issues. Hydrogen storage in the safest and most efficient solid material can reduce problems. Material has a great influence on human life. In the era of nanotechnology, microscopic analysis methods can investigate physical phenomena at the molecular level. [1]. In experiments show that large amounts of metal can form icosahedral structures in a liquid state [2]. The nature of crystals in silica gel is very interesting to study. Silica can be heated to 3500K with a cooling rate of $10^{14}$ K / s silicon [3]. Research on the icosahedral structure by simulation is also carried out on alloy material. Some materials such as Cu₈₀Si₂₀ using Ab Initio Molecular Dynamics [4] and CU-CO use molecular dynamics [5]. Research to study the structure of icosahedral formation in the event of changes in the solid-liquid-solid phase using the molecular dynamics method [6]. Through this research, important characteristics were investigated in the formation of icosahedral structures using molecular dynamics simulations.

2. Research Method
The method used in this research uses a literature study to get a theoretical basis for the dynamics of protons and hydrogen bonds. In this study using a numerical approach to solving proton motion equations with computational programs. Molecular dynamics simulations in this study use the Lennard-Jones equation and the percentage of icosahedral structures in the interaction of hydrogen and silica
gel. Calculation of molecular dynamics simulations using the Lennard-Jonnes equation [7] is shown in equation (1) and the percentage of icosahedral structures in equation (2)

\[
U = 4\varepsilon \left\{ \frac{\sigma^6}{r^6} - \left( \frac{\sigma}{r} \right)^{12} \right\} 
\]

(1)

\[
\text{% icosahedral} = \frac{\text{sum structure}}{\text{sum atom}} \times 100\%
\]

(2)

In this simulation the data is regulated in a temperature change from 2400K to 3200K. Temperature is made at a pressure of 2 Atm. In this simulation silica gel in silanol groups with a susceptible pore size of 2.4 Å to 2.8 Å.

3. Result and Discussion

In this study, temperature variations were carried out on the absorption of hydrogen on changes in the pore size of the silica gel. The simulation is run with an initial temperature of 2500K, 2625K, 2750K, 2875K, 3000K and 3125K to obtain changes in the Icosahedral structure in the liquid phase. The pore size of silica gel was taken at 2.4 Å, 2.6Å and 2.8Å. At a pore size of 2.4 Å, there is a change in% ico with a change in temperature shown in figure 1. At 2750K, the lowest ico% obtained was 0.6% in the formation of icosahedral structures and is still solid. At 3000K, the highest ico% of 1.4% showed that the absorption of hydrogen in silica gel could take place so that the icosahedral structure was formed in a liquid state.

![Figure 1. Changes in icosahedral at pore size of 2.4 Å with respect to temperature](image)

At a pore size of 2.6 Å, there was a change in% ico with the temperature change shown in figure 2. At 2875K, the highest% ico obtained by 1.4% shows that the absorption of hydrogen in silica gel can take place so that icosahedral is formed in a liquid state. In figure 2 shows the icosahedral changes
increase with temperature changes up to 2875K. The icosahedral decreases after this temperature but is not as significant as when increasing.

![Figure 2](image)

**Figure 2.** Changes in Icosahedral at a pore size of 2.6 Å with respect to temperature

At a pore size of 2.8 Å, there was a change in% ico with the temperature change shown in figure 3. At 2750K, the highest% ico obtained at 1.2% shows that the absorption of hydrogen in silica gel can take place so that icosahedral is formed in a liquid state. The icosahedral changes very quickly from an initial temperature of 2500K to 2750K, then decreases slowly as the temperature increases. If observed from the results of the simulation graph above, the initial cooling temperature of 2875K with a pore of 2.6Å is good enough for icosahedral to the hydrogen of 1.4%.

![Figure 3](image)

**Figure 3.** Changes in Icosahedral at pore size 2.8 Å with respect to temperature
4. Conclusion
We have successfully obtained the value of icosahedral silica gel which is adsorbed by hydrogen. At 2.4 Å pore size there is an icosahedral change of 1.4% at 3000K. At 2.6 Å pore size there is an icosahedral change of 1.4% at 2875K. At 2.8 Å pore size there is an icosahedral change of 1.2% at 2750K. From the results of research temperature changes at a pore size of 2.6 Å addressing that icosahedral takes place stably in the adsorption of hydrogen in silica gel. We observe that temperature affects the icosahedral process in silica gel.

Acknowledgments
Thanks to STITEK Bontang through LPPM STITEK Bontang in supporting the research that has been done. Research with grant number No.005 / LPPM / S-LT / 2019. Thank you also to all those who have helped with this research.

References
[1] Satoh A 2011 Introduction to Practice of Molecular Simulation Japan Akita Prefectural University
[2] Zetterling F 2003 Phase Transformations in Computer Simulated Icosahedrally Ordered Phases, Royal Institute of Technolgy
[3] Pamungkas M A and Widiyatmoko 2017 Jusamil Indonesian Journal of Materials Science 18 123–128
[4] Wu S, Kramer M J, Fang X W, Wang S Y, Wang C Z, Ho K M and Chen L Y 2012 Intermetallics. Elsevier 30 122-126
[5] Guo-Jian L, Qiang W, Tie L, Dong-Gang L, Xiao L and Ji-Cheng H 2009 Chinese Physics Letters 26 036104
[6] Hauwali N U J, Arkundato A and Rohman L 2016 Jurnal Ilmu Dasar 17(1) 19–24
[7] Fatriansyah J F, Dhaneswara D, Abdurrahman M H, Kuskendrianto F R, and Yusuf M B 2019 IOP Conference Series: Materials Science and Engineering 478 12034