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Thermal Conductivity of Liquid Lead for the Fast Nuclear Reactor Coolant, Calculated by the Green-Kubo Method Using Molecular Dynamics Simulation

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Abstract: Comprehensive information about nuclear reactor coolant materials for application in heat-transfer systems is very important. One important physical property that needs to be known is the thermal conductivity. The goal of this work is to predict the thermal conductivity value of the liquid lead, which is one of the important candidates for cooling materials for Gen-IV fast nuclear reactor designs. The thermal conductivity of liquid lead in this study was predicted using the Green-Kubo scheme and the molecular dynamics (MD) computational method to collect the simulation data. The MD simulation was done in the NVT ensemble, using the Lennard-Jones interaction potential. We observe the thermal conductivity of the liquid lead can be studied based on the diffusion physical process. The thermal conductivity of the liquid lead obtained from this research is $\lambda = 0.0113T + 8.8539$ [W/mK]. As a conclusion, this result is very suitable, compared with the available experimental data, then the Green-Kubo method can be used to calculate the thermal conductivity of liquid metal as lead.

Keywords: Green-kubo; Molecular dynamics; Molten liquid lead; Thermal conductivity

Introduction

Thermal conductivity is one of the important material properties that allows technological engineering with the right materials according to the application. Thermal conductivity defines how easily heat can move through a material. Materials that easily conduct heat, such as copper, are ideal for heat sinks, whereas materials with low thermal conductivity, such as ceramics, are ideal for thermal insulation (Xometry, 2023).

Computational thermal conductivity calculations (simulations) had previously been carried out for example for Argon gas in solid form, resulting in differences of up to a factor of 2 with the results of experimental measurements (Kaburaki et al., 1998). More recent research was conducted by Tretiakov et al. (2004), but it was reported that the measurement results still had a difference with experimental values. This is by the Lennard-Jones liquid results which have a difference of around 10% with experimental work over a relatively wide temperature range (Vogelsang et al., 1987). Calculations of physical quantities, such as thermal conductivity using molecular dynamics simulations, are greatly influenced by the potential interaction parameters between atoms of the material. Therefore, in applying the molecular dynamics simulation method, the best possible parameters must be obtained. Thermal conductivity calculations were also reported to be calculated for other solids by Jund et al (1999).

Thermal Conductivity of Liquids and Gases. According to physics, a fluid is a substance that easily (continuously) changes shape (flows) according to the shape of its container. The distance between molecules is much greater and the movement of molecules is more random in the liquid state than in the solid state so heat energy transport is less effective. Therefore, the thermal conductivity of gases and liquids is generally smaller

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than that of solids. However, because liquids/gases can move more easily than solids, they are very good for use in certain applications such as for heat transfer systems in nuclear reactors in the form of what is often called a coolant. Thermal conduction of a liquid (gas) is caused by the diffusion of its atoms or molecules from a higher energy level (temperature) to a lower energy level (temperature).

In this research, the thermal conductivity of a liquid metal system, namely liquid lead, will be calculated using the molecular dynamics simulation method. In liquids, the thermal conduction mechanism is caused by the diffusion process of atoms or molecules, but the physical mechanisms to explain the actual thermal conductivity of liquids are not yet well understood, although this quantity can be calculated. Liquids tend to have better thermal conductivity values than gaseous materials, and because of their flowability compared to solids, liquids are very suitable as a medium for transferring/removing excess heat from one place to another, as happens in nuclear reactors. This heat can be removed by channeling the liquid through a heat exchanger. The coolant used in nuclear reactors to transfer heat today is generally water or liquid metal, such as sodium or lead. However, the thermal conductivity of nonmetallic fluids generally decreases with increasing temperature so reactors operating at very high temperatures may be less suitable (Material Properties, 2023).

The reactor coolant is used to take heat from the fuel elements in the reactor core (the result of the fission reaction) and bring it to the boiler unit where the heat is released into water carried through the pipe system to convert it into steam. This steam will of course be used to rotate the electric generator turbine system. The efficiency of this process depends on the coolant flow rate, the flow cross-section of the fuel element, the temperature difference between the cladding and the coolant, and the choice of fuel coating material. The fuel and cladding must be designed so that they are capable of operating at the highest temperatures efficiently and safely. Likewise, this coolant is heated to the highest acceptable temperature (as the reactor operating temperature) to increase plant efficiency by providing steam to the turbine at high temperature and pressure. Reactor coolant materials, therefore, need to have several important characteristics such as chemically compatible and non-corrosive to heat transfer system materials, cheap and easy to obtain in a pure state, stable against radiation, clear state of matter, and high boiling point, ability to transfer high heat (thus high thermal conductivity), easy to move in the pump system. Of course, no coolant that meets all these requirements, and each coolant has one or several disadvantages compared to others according to the application objectives or nuclear reactor design (Collier, 2011).

Based on the background above, in this research, the thermal conductivity of one of the reactor coolants, namely liquid lead, will be studied. Liquid lead is one of the important candidates for the cooling material for GEN-IV nuclear reactors, namely liquid lead-bismuth cooled fast reactors (Pioro, 2023). The GEN-IV reactor design has at least 6 types of future reactor designs as a replacement for the traditional reactor designs that are currently operating. Until now, it is still in the development stage and nothing is ready to operate commercially.

In this preliminary computational research, the thermal conductivity of liquid lead will be calculated using the molecular dynamics method. The interaction potential between the atoms that make up liquid lead will be described using the Lennard-Jones potential as a simplification. The theory for calculating thermal conductivity will use the Green-Kubo method. The molecular dynamics code will use the code developed by Cheong (2004).

This research is important because the physical properties of reactor coolants must be well known, including the thermal conductivity of the material. If we want to find new potential materials for use as candidates for more efficient and safe reactor coolants, then a new material must be predictable for its physical properties before it is actually made in the laboratory. In this case thermal conductivity is not so easily calculated with good accuracy compared to experiments. In this study, the thermal conductivity calculation using the Green-Kubo method have been done. The challenge is if the results are very good, it can be used to calculate other reactor coolant candidates that have not been made in the laboratory

Method

Potential Lennard-Jones Interactions

One potential model of interaction between atoms of a material system, although very simple, is the Lennard-Jones (LJ) potential. Although this potential model is simple, for some cases, especially liquids and gases, it often produces quite good calculation results. Arkundato et al have used this LJ potential model to predict the value of the diffusion coefficient for solid-liquid metal systems with very good results by making several modifications to the method of calculating potential parameters for pairs of different types of atoms for metal systems (Arkundato et al., 2022). This LJ potential form is generally expressed analytically as Equation (1).

$$\phi(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \quad (1)$$

In Equation (1), the potential parameters *s*and *e* respectively describe the minimum distance r_{ij} that two atoms can be closer to each other (length units Å or meters) when interacting, the amount of attraction between two atoms that are close together within a distance r_{ij} (in energy units eV or joules). Plot Equation (1) above for any parameters sand e is in Figure 1.

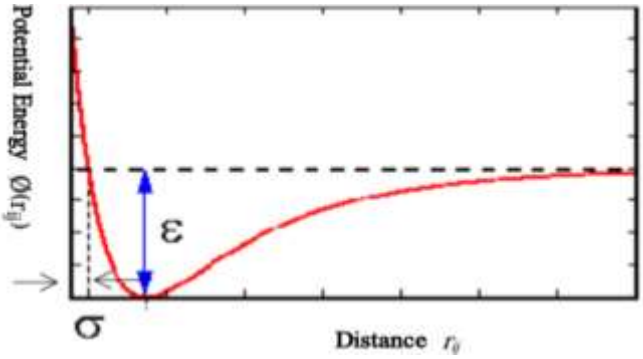

Figure 1. Lennard-Jones potential image

The application of the molecular dynamics simulation method to describe the physical processes that occur as reflected by the related physical quantities is carried out by calculating particle motion trajectories for systems of many particles interacting with each other based on certain interaction potentials, for example, using the LJ potential in Equation (1). The trajectories of these particles can be calculated based on the solution to Newton's equation of motion *F* = *ma* and by applying the concepts of Statistical Physics you can later calculate the physical quantities you want to know such as thermal conductivity. Currently, with the increasing development of computer and software capabilities, many molecular dynamics simulation computer programs have been created and developed. There are several that are popularly used such as LAMMPS (Thompson et al., 2022), MOLDY ((Refson, 2000), and a simple NVT program (which we used in this research) for thermal conductivity computation developed by Cheong (2004). In this program code, the thermal conductivity calculation facility has been developed and at the end of the simulation, we can know the value of the thermal conductivity of the material being simulated.

The physical quantity thermal conductivity is defined as a linear coefficient connecting the macroscopic heat flow J with the temperature gradient (Fourier's law):

$$\mathbf{J} = -\lambda.\nabla T \quad (2)$$

In this study, we calculate the thermal conductivity lambda λ using the Green-Kubo formula:

$$\lambda = \frac{1}{3Vk_BT^2}\int_0^{\infty}\langle \mathbf{j}(0)\mathbf{j}(t)\rangle dt \quad (3)$$

where *V* is volume and *T* is temperature or temperature.

Simulation Method

Argon at high temperatures (gas phase) can be well described by the LJ interaction potential which assumes an atom is a hard sphere. To calculate thermal conductivity, you can use the Green-Kubo approach or method to calculate the motion trajectories of atoms during the simulation. These methods generally require long running times (>106 time steps) to properly accommodate statistical effects (Cheong & Zheng, 2004). This LJ potential, although simple in form, also allows us to be used as an initial prediction for calculating physical quantities because the computational time scales quadratically with the size of the system. In this research, molecular dynamics simulations use the NVT code created with the Fortran program and can be downloaded from the website (Cheong & Zheng, 2004). This NVT molecular dynamics simulation program requires input in the form of:

```
! input.par MD_NVT simulation
2.5             ! cutoff
1.3422          ! density Pb      in the reduced units
0.284           ! temperature     in  the reduced units
1000000         ! MD steps using the Verlet integration
0.002           ! step size
100             ! quench_interval
100             ! quench_times
1000            ! write_scaler
```

The lead atoms are prepared into the FCC crystal lattice at the beginning of the simulation (by the NVT program code automatically) and assigned a moving speed based on a Gaussian distribution. Integration of Newton's equations of motion to obtain particle trajectories using the Verlet algorithm which is already popular in molecular dynamics methods. The initial material system for the simulation is initially solid and then given energy based on a Gaussian distribution to reach the temperature T as desired in the simulation. The interaction potential that we use is the Lennard-Jones potential. The integration time step is every 0.002 units. Verlet integration is carried out for 1000000 steps to get fairly accurate results. The output of this simulation is the material thermal conductivity value (lambda) at a

certain temperature T which can be seen in one of the output files after the simulation ends. The actual final temperature is expressed in K (kelvin) while thermal conductivity is expressed in $Wm^{-1}K^{-1}$ units.

Result and Discussion

Simulation Input Set-up

Thermal conductivity calculations for various temperatures were carried out using the Lennard-Jones potential with the NVT ensemble for 108 Pb lead atoms with Lennard-Jones potential parameters which can be entered in the NVT code in the Fortran language (NVT.f) before program compilation. Compiling the NVT.f program produces a .exe file. Running the NVT.exe program requires program input in the form of the input.par file. The LJ potential parameters for the Pb lead atom are using the values reported by Zhen and Davies (1983). The LJ interaction parameter values are sigma = 3.1888 Å (which must be converted to meters) and epsilon = 0.191 eV (which must be converted to joules). With these values, the command line in the NVT.f program that must be corrected is as follows:

```
!.....
! Command line in Fortran inside the NVT.f code
PARAMETER (sigma = 3.188D-10)
PARAMETER (eps = 3.06013367140902D-20)
PARAMETER (kb = 1.38062D-23, mass = 3.4406366D-25)
! massa Pb in kg units =  6.6335209E-26 kg
! sigma in meter units
! eps in J units   = 3.06013367140902D-20 K
! read parameters from qid.par.
!
! format of the qid.par file:
! rcut
! rho  in the reduced units = N x rho x sigma^3/V  = ....
! estimated with the packmol program for V volume
! temp, reduced units ={Kb x T}/eps   = 0.584  T =  70K
! nstep
! tstep
! quench_interval
! quench_times
! write_scaler
! .....
```

In this research, all simulations were carried out on a computer with the Linux Ubuntu operating system with the Fortran program used being Fortran 77 so that the NVT.f program was compiled on the Linux terminal using the command:

```
$g77 NVT.f -o NVT.exe
```

The number of atoms can be set in the NVT.f code, which in this simulation uses 108 Pb atoms. Figure 2 is an example of the configuration of lead material atoms at a certain temperature *T* (using the OVITO visualization program) (Stukowski, 2010).

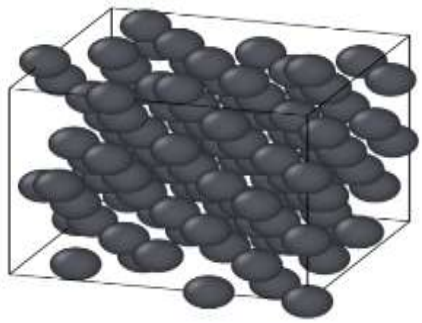

Figure 2. FCC crystal system for liquid lead

Thermal Conductivity Simulation Results

Table 1 summarizes the conversion from the SI units to the reduced units for the NVT ensemble molecular dynamics simulation input used in this study.

Table 1. Conversion Values for Simulation Input

T [K]	T (reduced)	Density [mol/L]	Density (reduced units)
600	0.2707	68.3169	1.3330
700	0.3158	69.8190	1.3623
800	0.3609	71.3211	1.3916
900	0.4061	72.8233	1.4209
1000	0.4512	74.3254	1.4502

Then after NVT simulation at each temperature and density for 1000000 Verlet integration steps with a meshtime of 0.002, the thermal conductivity (lambda) is obtained as in Table 2.

Table 2. Thermal Conductivity from Simulation Result

Temperature T[K]	Thermal Conductivity λ [W/mK]
629.47	15.96
729.21	17.00
820.08	18.18
908.74	19.06

Then, if we look for the relationship between the thermal conductivity values in table 2 above in the form of an analytical function using linear interpolation, we will get a graph like the one in figure 3.

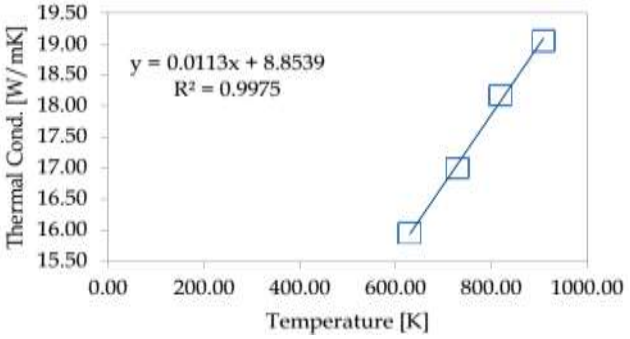

Figure 3. Thermal conductivity as a function of temperature

Dependence of Thermal Conductivity on Temperature

It is from figure 3 above, we get a formula for the thermal conductivity of molten lead as a function of temperature as in equation 4.

$$\lambda = 0.0113T + 8.8539 \ \text{[W/mK] (simulation)} \quad (4)$$

Now we compare the simulation results with the results of experiments carried out by other researchers. Sobolev et al have reported experimental work on liquid Pb conductivity values as a function of temperature in 2007 (Sobolev, 2007). In his report, he stated that the linear function of the thermal conductivity of molten lead is expressed by

$$\lambda = 0.011T + 9.2 \ \text{[W/mK] (experiment)} \quad (5)$$

where this correlation function can be used at temperatures up to T = 1300 K. If we express in graphical form the two functions of Equations (4) and (5) we get the following figure 4.

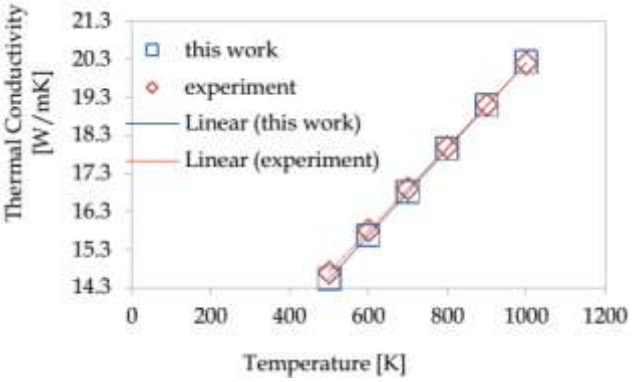

Figure 4. Comparison between two methods

It is from Figure 4 above, it is very clear that the prediction of the thermal conductivity of liquid lead which was carried out using the molecular dynamics method based on the Green-Kubo calculation method is very accurate, in accordance with experimental results, even for predictions at very high temperatures. This is important considering that many future nuclear reactors are designed to work at high temperatures and output power. Therefore, the Green-Kubo method has the potential to be used to predict the thermal conductivity of new materials that have not been discovered or have not been explored as potential candidates for better cooling media, in accordance with the requirements for reactor cooling materials as mentioned in the introduction. Some potential cooling materials are liquid metal alloys such as PbBi, PbLi, PbBiLi, and so on, allowing their properties to be studied using the Green-Kubo ensemble NVT molecular dynamics simulation method.

Research on reactor coolants from liquid lead (Pb) is very important because in the future understanding the characteristics of liquid lead will be very important in efforts to design fast type reactors which are among the popular designs for future reactors. Research on reactor design has been around for quite a long time, but research on the cooling potential of the reactor itself is also very important. Some of the preliminary researches are carried out by Su'ud (2008), Imron et al. (2010), and Krisna et al. (2012). They learn about the Small Pb-Bi Cooled Nuclear Power Plant Reactor.

Molecular dynamics simulation research on liquid lead coolant has also been carried out previously by some researchers, but instead of calculating thermal conductivity, it calculates the diffusion coefficient. Imanullah et al. (2018) simulated the temperature dependence of the liquid lead density by molecular dynamics simulation. Nuris (2019) studied the diffusion model of iron in liquid lead. Then, Ramadany et al. (2022) observed the effect of liquid lead onto the FeNi steel computationally using molecular dynamics simulation method.

However, lead is a heavy metal that is dangerous for the body if it is accidentally absorbed into body tissues. Therefore, even though the use of liquid lead metal as a reactor coolant is very promising, it must be properly maintained because liquid lead vapor is very toxic and can be easily inhaled and can pollute the environment (Khairuddin et al., 2021; Siswoyo et al., 2018; Suprihatin et al., 2011).

From the results of this research, apart from producing the conclusion that the Green-Kubo method can be used to predict the thermal conductivity value of liquid metals, this research idea can be developed towards developing learning in the world of education. A dry lab can be developed to create a physics learning model in schools to improve understanding and mastery of physics concepts using molecular dynamics simulation methods with the help of computer equipment in computer laboratories at schools. Previously, some of effort to improve science process, understanding of physics concept with many learning

models have been developed by many researchers. Fitri et al. (2023) have implemented the REACT learning model on students. This model was also developed by Januarti et al. (2023) and also Salam et al. (2023). Anbiya et al. (2023) tried to integrate the problem-based learning models with guided inquiry worksheets to examine the improvement of students' scientific process skills and critical thinking abilities. Also, Yutia et al. (2023) developed teaching materials in the form of e-student worksheet with a scientific approach to static fluid material to improve critical thinking skills of the students. Then, Syam et al. (2023) used a virtual laboratory to develop a problem-based virtual laboratory. Liunokas et al. (2023) developed a dry lab model using audio analysis software to improve students' understanding of concepts about sound waves. More, the 2013 curriculum shows the important literacy skills in learning physics, and physics learning is always closely related to practicum. So, the use of dry lab should be important for physics student (Hidayati et al., 2023).

Conclusion

The thermal conductivity of liquid lead can be predicted using the Green-Kubo scheme, based on the molecular dynamic's simulation method. The thermal conductivity of liquid lead obtained from this research is $\lambda = 0.0113T + 8.8539$ [W/mK] with very good results compared to existing experimental results.

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Author Contributions

Simulation data, A.A.; Manuscript preparation, A.A.; Manuscript editing, R.D.S; Free plagiarism/Turnitin, W.M.; Computational facility, L.R.; Manuscript submission, W., A.A.; Manuscript revision, A.A.

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Conflicts of Interest

The authors declare no conflict of interest.

References

Anbiya, K., Muhibbudin, Khaldun, I., & Yusrizal. (2023). Integration of Problem-Based Learning Model with Guided Inquiry Worksheet to Enhance Scientific Process Skills and Critical Thinking Abilities. *Jurnal Penelitian Pendidikan IPA*, *9*(10), 8328–8334. https://doi.org/10.29303/jppipa.v9i10.4724

Arkundato, A., Monado, F., Sugihartono, I., Rivai, A. K., & Su'ud, Z. (2022). Diffusion coefficient calculation of iron in liquid lead using molecular dynamics method with new mixing rule for Lennard-Jones potential parameters. *Kuwait Journal of Science*, *50*(3B), 1–15. https://doi.org/10.48129/kjs.17205

Cheong, K. S. (2004). *Thermal Conductivity of Argon from the Green- Kubo Method*. Retrieved from https://courses.physics.illinois.edu/phys466/sp2013/projects/2004/Team1/index.html

Collier, J. G. (2011). Coolants, Reactor. In *A-to-Z Guide to Thermodynamics, Heat and Mass Transfer, and Fluids Engineering*. Begellhouse. https://doi.org/10.1615/AtoZ.c.coolants_reactor

Fitri, R., Nasir, M., & Fakhruddin. (2023). Efforts to Improve Science Process and Collaboration Skills with the Implementation of the REACT Learning Model on Students. *Jurnal Penelitian Pendidikan IPA*, *9*(10), 8301–8307. https://doi.org/10.29303/jppipa.v9i10.5170

Hidayati, H., Ningsi, A. W., & Iskandar, A. M. (2023). Design and Validity of Student Worksheet Integrated Scientific Literacy for The Use of Physics Practicum KIT. *Jurnal Penelitian Pendidikan IPA*, *9*(1), 384–389. https://doi.org/10.29303/jppipa.v9i1.2887

Imanullah, M. A. B., Arkundato, A., & Purwandari, E. (2018). Density of Liquid Lead as Function of Temperature and Pressure Based on the Molecular Dynamics Method. *Computational And Experimental Research In Materials And Renewable Energy*, *1*(1), 1. https://doi.org/10.19184/cerimre.v1i1.19541

Imron, Su'ud, Z., & Pasek, A. D. (2010). Source Term Calculation of Small Pb-Bi Cooled Non-Refueling Nuclear Power Reactor 20 MWe (SPINNOR 20MWe. *Indonesian Journal of Physics*, *21*(2), 61. https://doi.org/10.5614/itb.ijp.2010.21.2.5

Januarti, Islami, N., & Yennita. (2023). Development of Physics Modules Based on the REACT Learning Model of Sound Wave Material to improve the ability to Understand Concepts. *Jurnal Penelitian Pendidikan IPA*, *9*(10), 8489–8497. https://doi.org/10.29303/jppipa.v9i10.4393

Jund, P., & Jullien, R. (1999). Molecular-dynamics calculation of the thermal conductivity of vitreous silica. *Physical Review B*, *59*(21), 13707–13711. https://doi.org/10.1103/PhysRevB.59.13707

Kaburaki, H., Li, J., & Yip, S. (1998). Thermal Conductivity of Solid Argon by Classical Molecular Dynamics. *MRS Proceedings*, *538*, 503. https://doi.org/10.1557/PROC-538-503

Khairuddin, K., & Yamin, M. (2021). Analysis of Cadmium (Cd) and Lead (Pb) Heavy Metal

Content in Shell and Mangroves at Bima Bay. *Journal of Science and Science Education*, *2*(1), 58–61. https://doi.org/10.29303/jossed.v2i1.726

Krisna, D. N., & Su'ud, Z. (2012). Study Neutronic of Small Pb-Bi Cooled Non-Refuelling Nuclear Power Plant Reactor (SPINNOR) with Hexagonal Geometry Calculation. *Indonesian Journal of Physics*, *23*(1), 16–22. https://doi.org/10.5614/itb.ijp.2012.23.1.4

Liunokas, M. T., & Asbanu, D. E. S. I. (2023). Revolutionizing Physics Education: Enhancing High School Students' Understanding of Standing Wave Concepts through Mictester-Based Smartphone Experiments. *Jurnal Penelitian Pendidikan IPA*, *9*(10), 8563–8568. https://doi.org/10.29303/jppipa.v9i10.3771

Material Properties. (2023). *Thermal Conductivity of Materials*. Retrieved from https://material-properties.org/thermal-conductivity-of-materials/

Nuris, A. A. (2019). Modeling of Ferrous Metal Diffusion in Liquid Lead Using Molecular Dynamics Simulation. *Computational And Experimental Research In Materials And Renewable Energy*, *2*(1), 45. https://doi.org/10.19184/cerimre.v2i1.20561

Pioro, I. L. (2023). *Handbook of Generation IV Nuclear Reactors*. Elsevier. https://doi.org/10.1016/C2019-0-01219-8

Ramadhany, F., Misto, M., Mulyono, T., & Hasan, M. (2022). Interaction Between Liquid Lead and FeNi Material Using Molecular Dynamics Simulation. *Computational And Experimental Research In Materials And Renewable Energy*, *5*(1), 48. https://doi.org/10.19184/cerimre.v5i1.31477

Refson, K. (2000). Moldy: a portable molecular dynamics simulation program for serial and parallel computers. *Computer Physics Communications*, *126*(3), 310–329. https://doi.org/10.1016/S0010-4655(99)00496-8

Salam, A. A. K., Abdullah, H., & Amin, B. D. (2023). Development of REACT-Oriented Student Worksheets to Improve Physics Learning Outcomes. *Jurnal Penelitian Pendidikan IPA*, *9*(1), 462–471. https://doi.org/10.29303/jppipa.v9i1.2497

Siswoyo, E., & Habibi, G. F. (2018). Sebaran Logam Berat Cadmium (Cd) dan Timbal (Pb) pada Air Sungai dan Sumur di Daerah Sekitar Tempat Pembuangan Akhir (TPA) Wukirsari Gunung Kidul, Yogyakarta. *Jurnal Pengelolaan Sumberdaya Alam Dan Lingkungan (Journal of Natural Resources and Environmental Management)*, *8*(1), 1–6. https://doi.org/10.29244/jpsl.8.1.1-6

Stukowski, A. (2010). Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool. *Modelling and Simulation in Materials Science and Engineering*, *18*(1), 015012. https://doi.org/10.1088/0965-0393/18/1/015012

Su'ud, Z. (2008). Optimization of small and very small long life Pb-Bi Cooled Fast reactors. *Indonesian Journal of Physics*, *15*(2), 43–50. Retrieved from http://ijp.papsi.org/index.php/ijp/article/viewArticle/93%5Cnpapers3://publication/uuid/9F74B8D1-4FD2-484D-AA57-0C7F22009468

Suprihatin, S., & Indrasti, N. S. (2011). Penyisihan Logam Berat dari Limbah Cair Laboratorium dengan Metode Presipitasi dan Adsorpsi. *MAKARA of Science Series*, *14*(1). https://doi.org/10.7454/mss.v14i1.473

Syam, Y. R., Retnowati, R., & Kurniasih, S. (2023). Development of a Virtual Laboratory Based on Problems in the Circulatory System Matter. *Jurnal Penelitian Pendidikan IPA*, *9*(10), 8415–8421. https://doi.org/10.29303/jppipa.v9i10.5195

Tretiakov, K. V, & Scandolo, S. (2004). Thermal conductivity of solid argon at high pressure and high temperature: A molecular dynamics study. *The Journal of Chemical Physics*, *121*(22), 11177–11182. https://doi.org/10.1063/1.1812754

Vogelsang, R., Hoheisel, C., & Ciccotti, G. (1987). Thermal conductivity of the Lennard-Jones liquid by molecular dynamics calculations. *The Journal of Chemical Physics*, *86*(11), 6371–6375. https://doi.org/10.1063/1.452424

Xometry, T. (2023). *Thermal Conductivity: Definition, How It Works, Importance, Calculations, and Factor*. Retrieved from https://www.xometry.com/resources/materials/thermal-conductivity/

Yutia, N., Yusnaidar, & Hasibuan, M. H. E. (2023). Development of Electronic Student Worksheets with a Scientific Approach to Static Fluids Material to Improve Critical Thinking Skills of SMAN 9 Merangin Students. *Jurnal Penelitian Pendidikan IPA*, *9*(10), 8383–8389. https://doi.org/10.29303/jppipa.v9i10.5291