

Do Molecular Simulations Represent the Real World at the Atomic Scale? – A Spiritual Insight

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Molecular Simulations are used to model real world atomic scale problems so that we can gain a greater understanding of what is happening at the atomic scale. At a fundamental level, molecular dynamics simulations begin with Newton's equations of motion which form the basis for classical mechanics. Such software generally includes force-field methods for modeling the potential energy surfaces. These simulations may then be used to derive critical physical parameters that may be compared to experimental results for validation of the model.

References

1. *Katherine J. Harmon et al, **Validating first-principles molecular dynamics calculations of oxide/water interfaces with x-ray reflectivity data**, *Physical Review Materials* (2020). DOI: [10.1103/PhysRevMaterials.4.113805](https://doi.org/10.1103/PhysRevMaterials.4.113805)*

One of the advantages of computer simulation of materials is how these simulations offer a molecular level of understanding and insights into the engineering of green energy technologies. Such technologies include energy storage (batteries), solar energy usage, and CO₂ capture from important energy generation systems. In order for the computational modeling to be useful, the simulation needs to be validated in order to check whether the information the model provides is appropriate. In a recent research paper, [1] published in 2020 in the Physical Review Materials Journal, scientists used molecular dynamics to study the oxide/water interfaces coupled with experimental x-ray reflectivity data. The researchers were focusing upon solid-liquid interface in order to understand what is happening as water interacts with a metal oxide surface.

A team of researchers at the U.S. Department of Energy (DOE) Argonne National Laboratory, the University of Chicago, and the University of California Davis, developed a new validation protocol for simulations of the atomic structural changes during water interaction with a solid. This is why x-ray diffraction was utilized as the x-ray reflectivity data is capable of showing the structural changes at the surface during H₂O interaction. They state that most model validation protocols deal with bulk materials and ignore interfaces. The validation procedure they designed was using a high-resolution x-ray reflectivity measurement of an aluminum oxide-water interaction. This was conducted at the Argonne's Advanced Photon Source laboratory. The computational work was also performed on the Argonne Leadership computing facility supercomputer. The x-ray reflectivity data provides information on the interatomic distances which allowed researchers to directly probe the atomic surface structures during the solid-liquid interactions.

The validation protocol helps to elucidate the strengths and weaknesses of the computational simulations. This facilitates the building of more accurate models for future work. These simulations also provided new insights into the x-ray reflectivity data itself. The research work showed how the measurements are sensitive not only for the atomic positions, but also to the electron distribution surrounding each atom on the surface. This information provides more insight for future experimental and simulation work on solid-liquid interfaces.

The Spiritual Insights that we receive from this type of research is related to the validation process that we need for truth and righteousness. One of the key conclusions of postmodern culture is a rejection of the idea that objective truth exists. Truth is now regarded as a function of political and social power, and truth is used as a way to control a set of outcomes in one's life. This is why the social media tech giants and internet search engines work so hard at manipulating the masses through their algorithms which prevent people from seeing certain types of news/information. As living in a postmodern world, the lines of truth are blurred more and more today as more and more people struggle with knowing what is truth, especially in areas of gender and sexual preference, where human rationalism goes out the door. The Scriptures teach us starting from the Torah, that as God's children we are called to think counter-culturally. Paul teaching from the Torah speaks of not letting our minds be conformed to this world. (**Romans 12:2**) This means that we are not to allow our culture to squeeze our minds into a mold that models this world's set of truths. In **Romans 12**, Paul tells us ואי תדמו לעולם הזה "do not to be conformed to this world" using the word to be transformed דמה to translation the greek word **συσχηματίζω** meaning "*to fashion alike*" or "*conform to the same pattern (figuratively)*." The idea here is that we are changed on the inside as God's Word is powerful to change us, His truth is powerful, and as we hold to the truth of what God's Word states the Lord God Almighty will transform our hearts and our lives for His glory! This is what Paul meant when he said that we are to put on the mind of Messiah according to 1 Corinthians 2:16. Paul calls the evil one the god of this world because he blinds the eyes of those who do not believe so they cannot see the truth of God in the Messiah Yeshua. (**2 Corinthians 4:4**) Because the evil one is in charge and actively deceiving many people, this world, our culture, portrays lies on many fronts, propaganda, fear, lust, pride, anger, and the list could go on. We must be diligent to discern the truth even more so in this present age. The Scriptures function in a way so as to increase our faith, and knowledge of truth, and this is achieved through both the study of

God's Word and applying God's word to our lives! The Scientific research draws out this concept of our needing to test this world's set of assumptions against the truth that we find in the Scriptures.

When we consider these things, we know there are certain assumptions the world has that enter into the discussion. The world does not believe in the existence of God in Heaven. Therefore, the primary assumption is to the reliability and trustworthiness of the Scriptures. If we question why we should believe in the authority and credibility of Scriptures, we do so due to the historical experience of the people of Israel, including their origins as the descendants of Abraham, Isaac, and Jacob. Israel was enslaved in Egypt for 400 years, and delivered from bondage by the power of God in Exodus, and the Lord God desiring to dwell in their midst, revealed by the revelation of the Torah at Mount Sinai, etc. In addition to this, there was an intense scribal tradition in the preservation of the Scriptures, this is derived from the Torah according to Devarim / Deuteronomy 12:32.

ספר דברים פרק יג

א את כל-הדבר אשר אנכי מצוה אתכם אתו תשמרו לעשות לא-תסף עליו ולא תגרע ממנו:

DEVARIM / DEUTERONOMY 12:32

12:32 "WHATEVER I COMMAND YOU, YOU SHALL BE CAREFUL TO DO; YOU SHALL NOT ADD TO NOR TAKE AWAY FROM IT." (NASB)

The Lord God Himself commands us to be careful to obey His Word. This verse speaks to the necessity of our using God's Word for understanding truth and that we are not to change the truth. The followers of the God of Israel and His Messiah Yeshua are commanded to love the truth and to think clearly about their faith. We note what happened to those who hated the truth, "*people perish because they refuse to love the truth and so be saved.*" (2 Thessalonians 2:10). Those who reject the truth of God's Word remain spiritually dead (Tehillim / Psalms 78:22, John 3:36, Hebrews 3:18, 1 John 5:12). The Scriptures are full of the truth claims about the Messiah of God, as the one who comes to deliver God's people, and the Lord God according to the Scriptures describes Yeshua as the one who does this. The Lord God Almighty commands all people to believe this truth. (Acts 17:30-31, 1 Timothy 2:4). Because of this, we believe the truth of God is central to not just being saved but for the Lord God also working in our lives to do so. This means we must hold on to God's truth in our hearts, and apply His truths to our lives, in order to expect Him to work and dwell in our hearts and lives. Other worldviews, such as the postmodernism or liberal ideologies distorts the truth and prevents one from completely embracing the truth about the Messiah and God's Word. The greatest truth claim is found in the Shema according to Devarim / Deuteronomy 6:4-9.

ספר דברים פרק ו

ד שִׁמַע יִשְׂרָאֵל יְהוָה אֱלֹהֵינוּ יְהוָה | אֶחָד: ה וְאָהַבְתָּ אֶת יְהוָה אֱלֹהֶיךָ בְּכָל-לִבְבְּךָ
 וּבְכָל-נַפְשְׁךָ וּבְכָל-מְאֹדְךָ: ו וְהָיוּ הַדְּבָרִים הָאֵלֶּה אֲשֶׁר אֲנִי מְצַוְךָ הַיּוֹם עַל-לִבְבְּךָ: ז
 וְשָׁנַנְתָּם לְבְנֶיךָ וְדַבַּרְתָּ בָּם בְּשַׁבְּתְךָ בְּבֵיתְךָ וּבְלִקְתְּךָ בַּדֶּרֶךְ וּבְשֹׁכְבְךָ וּבְקוּמְךָ: ח
 וְקָשַׁרְתָּם לְאוֹת עַל-יָדְךָ וְהָיוּ לְטֹטְפֹת בֵּין עֵינֶיךָ: ט וְכָתַבְתָּם עַל-מַזְזוֹת בֵּיתְךָ
 וּבְשַׁעְרֶיךָ:

DEVARIM / DEUTERONOMY 6:4-9

6:4 'HEAR, O ISRAEL! THE LORD IS OUR GOD, THE LORD IS ONE! 6:5
 'YOU SHALL LOVE THE LORD YOUR GOD WITH ALL YOUR HEART
 AND WITH ALL YOUR SOUL AND WITH ALL YOUR MIGHT. 6:6
 'THESE WORDS, WHICH I AM COMMANDING YOU TODAY, SHALL
 BE ON YOUR HEART. 6:7 YOU SHALL TEACH THEM DILIGENTLY TO
 YOUR SONS AND SHALL TALK OF THEM WHEN YOU SIT IN YOUR
 HOUSE AND WHEN YOU WALK BY THE WAY AND WHEN YOU LIE
 DOWN AND WHEN YOU RISE UP. 6:8 'YOU SHALL BIND THEM AS A
 SIGN ON YOUR HAND AND THEY SHALL BE AS FRONTALS ON
 YOUR FOREHEAD. 6:9 'YOU SHALL WRITE THEM ON THE
 DOORPOSTS OF YOUR HOUSE AND ON YOUR GATES. (NASB)

These Scriptures reveal to us the importance of God's Word, that we are to listen to the Word of the Lord, we are to love him with all of who we are, and we are to teach God's Word to our children. Not simply teaching the Word of God, but actually living God's Word out in our lives. This is what it means when it says וְשָׁנַנְתָּם לְבְנֶיךָ וְדַבַּרְתָּ בָּם בְּשַׁבְּתְךָ בְּבֵיתְךָ וּבְלִקְתְּךָ בַּדֶּרֶךְ וּבְשֹׁכְבְךָ וּבְקוּמְךָ we are to speak of God's Word when we sit, when we stand, when we lay down, when we rise up, and when we walk along the way, etc, the way the text is written is descriptive of how pervasive the Word of God is to be in our lives. The Lord God Almighty created man to have the ability to comprehend truth, and to understand God's Word, and to discern between right and wrong. The existence of Israel and the Jewish people today, and the stories laid out in the Torah of Moshe are central to the message God has for all men, women, and children in this world that He wants to dwell in our midst, and deal with the problem of sin and death, to deliver us from judgement for sin. This was the purpose of the Lord God sending His redeemer Yeshua such that we can make the decision to believe and trust in the Lord God that He had done this for us.

The Torah prefigures what Yeshua would do, as explained in the sacrifices of the Tabernacle. We are told that blood was given to make atonement for our sins (Vayikra / Leviticus 17) demonstrated in the life-for-life concept of atonement. The one who was in a covenant relationship with God would place his hand upon the head of a sacrificial animal, confessing his sins, while the animal was slaughtered in his place. The most significant aspect of this is that the text speaks of a man or woman, who are already in a covenant relationship with the Lord, are to bring the sacrifice, a life for a life. This means bringing a sacrifice was not a means for one earned his own salvation. These commands were for those who were already redeemed, and belonging to the God of Israel, who were in a covenant relationship already, standing before the God that they loved the God who granted mercy and grace to be saved,

to repent, and even to have faith to obey God's Word! Granted, there were men in the history of Israel who thought by their simply bringing a sacrifice before the Lord they were good to go. However, we know the Torah does not teach a works based salvation as modern theologies today suggest. The Lord God Almighty said through His prophets over and over again how he desires mercy rather than sacrifice (1 Samuel 15:22-23, Mishley / Proverbs 21:3, Tehillim / Psalms 51:6, Jeremiah 7:21-23, Micah 6:8, Matthew 12:7), illustrating the sacrifices were meant to be for those who loved the Lord and who were already redeemed and in a covenant relationship with God! This demonstrates why modern theologies today are in such great error (i.e. dispensationalism) when teaching a lie that man earned his salvation in the OT. This is not what the Scriptures teach us, and this is why it is so important that we understand the difference between teaching a theology as opposed to teaching what the scriptures actually say! These things prefigured, or illustrated how the blood of the Messiah would purify us from sin. These things are related to the Torah centric principle of "making the one who did not know sin to be sin for us so that in him we would become the righteousness of God" (2 Corinthians 5:12, Galatians 3:13, 1 Peter 3:18). The death of the Messiah reveals the heart of God's Word to His people! In the Messiah we find the restoration of relationship of the people to the Lord, a restored life, and building of faith in God for the atonement from sin in the blood of Yeshua. What Yeshua did demonstrates the holiness and absolute regard for the truth of God, while at the same time extending His compassion to those who trust in Him. (Romans 3:26) The Lord God of Israel is the one who justifies all of those who trust in His redemption. These things speak to our needed to receive the miracle of life from above, until we do so we are spiritually dead and not able to understand what the Scriptures are telling us about who we are and about the Love of God who saves and delivers us out of bondage!

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Dr. Duane D. Miller received his Ph.D., M.S., and B.S. Degree in Chemical Engineering from The University of Akron Ohio. He is currently a Chemical Engineering Researcher. Duane's research expertise has focused upon functional materials development for the control, conversion, and release of process gases in Energy production technologies. His R&D interests include computational chemistry, developing novel technologies for converting biomass to fuels and studying their fundamental interactions during the chemical conversion process. His past experience includes sorbent development for pre- and post-combustion CO₂ and SO₂ capture, selective absorption of H₂S from methane streams, O₂ capture for oxy-fuel combustion, photocatalytic reduction of alcohols, NO_x reduction catalysis, the development of oxygen carriers to combust fossil fuels (CH₄ and coal) for the chemical looping combustion processes, and the extraction of rare earth elements using patent pending sorbents. His research expertise has focused on operando-characterization using Infrared, Raman, and UV-Vis spectroscopy to observe the nature of the catalytic active sites and reaction intermediates under realistic reaction conditions, allowing direct correlation of molecular/electronic structures with catalyst performance during Gas-Solid / Liquid-Solid Adsorption and Photocatalytic Processes with real time online analysis of reaction products using ICP-MS and mass spectrometry. His current work involves a multi-disciplinary approach to developing, understanding, and improving the catalytic gasification of coal and methane, high temperature chemical looping combustion, and the catalytic decomposition and gasification of biomass and coal using novel microwave reactor. He has been studying the Hebrew Scriptures and the Torah for 20+ years and sharing what he has learned. The studies developed for MATSATI.COM are freely to be used by everyone, to God be the Glory!

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