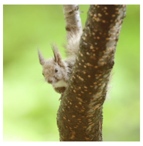
科学が物語へと変わるとき



若　者

Harry Handoko HALIM*

When Science Becomes a Story

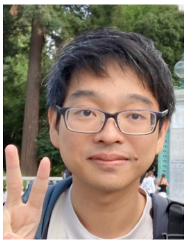
Key Words: Story, theory-experiment, material science, humanity, endeavor

日本語要旨

私は、科学研究を単なる知識の集積ではなく、「物語」として捉えている。研究とは、好奇心に導かれ、迷い、試行錯誤しながら意味を見出していく過程であり、優れた物語と同じように、人の理解や記憶に深く残るものだと感じている。科学は答えを与えるだけでなく、世界と私たち自身の位置づけを考える手がかりを与えてくれる。

私の専門である物質科学では、原子の初期状態や最終状態は高精度で捉えられる一方、その間に起こる連続的な運動は直接観測が難しい。この「見えない時間」こそが本質的な物理・化学現象の舞台である。分子動力学シミュレーションと機械学習ポテンシャルの進展によって、私は原子の動きを時間軸で追跡し、触媒反応のような複雑で動的な過程を可視化できるようになった。

こうした手法は、理論と実験の間に横たわる溝を埋める。静的な数値の比較ではなく、「ふるまい」を共有できる点に、私は大きな可能性を感じている。同時に、研究とは不確実性と向き合う人間的な営みでもある。回り道や停滞も物語の一部だ。自然が語る物語と、私たちが紡ぐ物語の両方に向き合いながら、私はこれからも意味ある科学の物語を描いていきたい。



* Harry Handoko HALIM
1996年12月生まれ
The University of Osaka Graduate School of Engineering Department of Precision Engineering Morikawa Laboratory（2023年）
Assistant Professor Doctor Material science
TEL：06-6879-7288
E-mail: harry@prec.eng.osaka-u.ac.jp

Of all things in this world, what I like the most is story. That is why I am drawn to research as it has the ability to unfold as a story—one that is not only engaging, but genuinely enjoyable to follow. Like a good story, research draws us in with curiosity, rewards patience, and gives meaning to moments of uncertainty. Science does not simply deliver answers; it helps us make sense of the world and our place within it. When research works well, abstract ideas become something we can share, discuss, and remember. In this way, storytelling is not separate from science, but one of the ways science becomes meaningful for humanity. I believe that even the most abstract mathematics can be understood and communicated through a compelling story.

There are two kinds of stories that can unfold in science. One is *intrinsic*: the story written by nature itself, describing how matter moves, interacts, and transforms according to principles that exist independently of us. The other is *extrinsic*: the human story constructed through research, shaped by our questions, limitations, hard work, and imagination. Research becomes most compelling when these two levels reinforce one another. In this article, I would like to share how my own research seeks to foster this alignment, allowing intrinsic and extrinsic stories to emerge together. I believe this perspective can be found across many scientific fields, but I will describe it here from my own standpoint as a materials scientist.

The Intrinsic Story

Despite remarkable advances in experimental and theoretical techniques that allow us to characterize matter with extraordinary precision, the true nature of atomic motion often remains elusive. We can capture initial and final states with high accuracy, yet what happens in between—the continuous, dynamic movement of atoms—remains difficult to observe directly. It is like cooking while knowing the recipe and tasting the final dish, yet never seeing how heat, time, and interaction transform the ingredients in between. In many cases, it is precisely within this hidden interval that the most important physics and chemistry unfold.

Advances in simulation techniques have opened new ways to address this challenge. Researchers can now follow how atoms move and interact over time, at scales that were previously difficult to observe. Instead of relying only on isolated snapshots or numerical results, these simulations allow us to watch materials evolve continuously—almost like viewing a "molecular movie". This is made possible through *molecular dynamics simulations*, in which the motion of atoms is calculated step by step according to physical laws, allowing their trajectories to be followed as time progresses.

Molecular dynamics itself is not a new idea. It has been developed and refined over several decades and has long served as a powerful tool for understanding the motion of atoms and molecules. However, traditional molecular dynamics simulations face important limitations. Accurately describing atomic interactions requires detailed physical calculations, which restricts simulations to relatively small systems and short time scales. As a result, many real-world phenomena—such as slow structural changes, rare events, or collective behavior involving thousands or millions of atoms—have remained difficult to capture directly.

Recent developments in *machine-learning interatomic potentials* have begun to change this situation. By learning atomic interactions from high-quality reference data (**Figure 1a**), these models retain much of the accuracy of fundamental physical descriptions while dramatically reducing computational cost. This makes it possible to simulate larger systems over longer periods of time, bringing simulations closer to the spatial and temporal scales of real materials. In doing so, molecular dynamics can now address complexity that was previously out of reach, allowing theoretical models to engage more directly with the conditions under which experiments are performed and phenomena unfold in reality.

To make this idea more concrete, **Figure 1(b-d)** presents an example from my own research, illustrating how atomic motion on a catalytic surface can be followed explicitly in time. By moving beyond static structures, the simulation captures how surface atoms and adsorbed molecules move, interact, and respond dynamically under reaction conditions. This ability to observe continuous atomic motion is essential for revealing the *intrinsic story* of the system—how catalytic activity emerges naturally from atomic-scale processes rather than from isolated snapshots. In this sense, the figure serves not only as a result, but as a way of understanding how the system truly behaves.

I find this shift particularly compelling because it changes how complex phenomena are understood. When atomic motion can be followed in time, it no longer feels abstract or detached from intuition. We can see how atoms rearrange, how bonds form and break, and how collective behavior emerges from simple interactions. For me, this storytelling aspect of simulation is not merely aesthetic; it reshapes how understanding itself is formed, bringing us closer to both the intrinsic story of nature and the extrinsic story of human inquiry.

This way of seeing is especially important in my own research on surface science related to catalysis. Catalytic processes are inherently dynamic: surface structures fluctuate, adsorbed molecules migrate, and

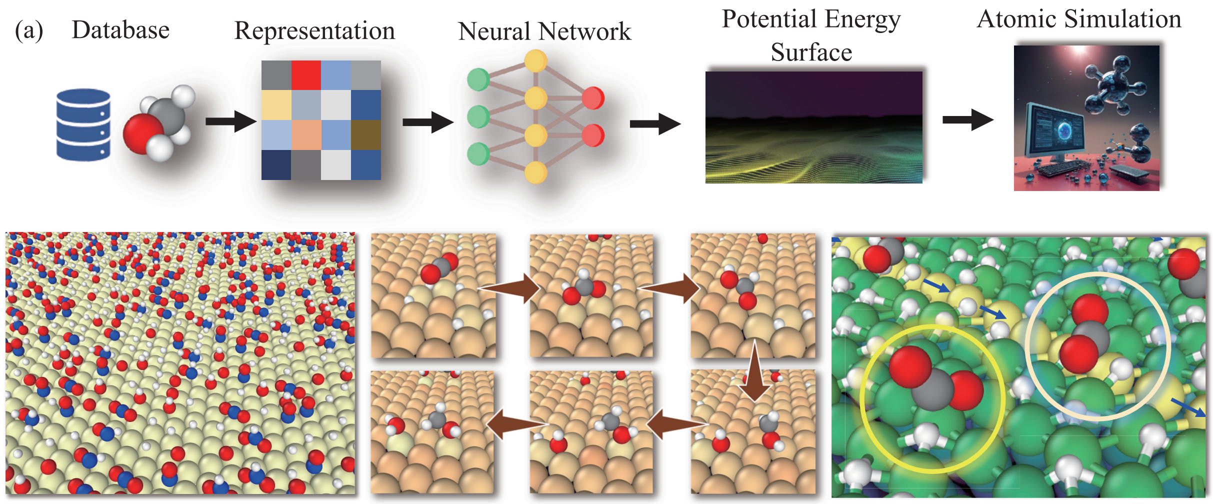


Figure 1. Illustration on how atomic-scale simulations can be used to reveal the dynamic nature of catalytic processes. Panel (a) presents a schematic overview of machine-learning-based atomic simulations. Panel (b) shows a catalytic surface populated with adsorbed species, while panel (c) depicts the reaction pathway of CO_2 *hydrogenation leading to methanol formation. Panel (d) highlights how hydrogenation proceeds on a dynamically evolving surface, where surface reconstruction occurs under hydrogen exposure.*

reaction pathways evolve in response to their environment. By explicitly following atomic motion through simulation, I aim to capture these coupled processes within a unified framework, allowing theoretical models to approach the complexity of real catalytic systems more closely than static calculations alone.

Beyond revealing the intrinsic story of atomic motion, these approaches also create a powerful connection between theory and experiment. Traditionally, the two have often felt separated: experiments probe realistic conditions but can be difficult to interpret at the atomic level, while theory offers interpretation but is constrained by idealization and computational cost. Multi-scale simulations like Molecular Dynamics help bridge this gap by enabling theoretical models to operate at experimentally relevant scales. Instead of comparing isolated structures or energies, theory and experiment can now discuss behavior—how systems evolve in time.

This relationship between observation and interpretation has deep historical roots. It reminds me of the collaboration between Tycho Brahe and Johannes Kepler. Brahe was an extraordinary experimentalist who devoted his life to precise astronomical observations, compiling an unprecedented body of reliable data. Yet he lacked the theoretical framework needed to fully interpret what he had measured. Kepler, by contrast, was a theorist with profound mathematical insight, but without Brahe's meticulous observations his ideas would have remained speculative. It was only through their combined efforts that the laws of planetary motion emerged, fundamentally reshaping our understanding of the universe.

In many ways, modern research faces a similar situation. Experiments show us how real systems behave, while theory helps us understand the underlying principles. Multi-scale simulations supported by machine learning help connect these two by allowing theory to work with conditions closer to those of experiments. Rather than replacing either approach, these methods help experiments and theory communicate more effectively, resulting in good dialogue and enjoyable conversation.

The Extrinsic Story

The extrinsic story of research goes beyond methods and techniques. Research is often described as a series of successes, but the real experience is rarely straightforward. Much of it involves uncertainty: calculations that do not work as expected, results that are hard to understand, and long periods when progress is difficult to see. If research were described as a novel, I would see it as an adventure story, where each project follows its own journey filled with detours, challenges, and unexpected events. Yet as long as we keep moving forward, the journey will reward us with meaningful treasures.

Research does not only require technical skill, but also patience and comfort with uncertainty. A memorable example for me is the story of Ludwig Boltzmann. He devoted much of his life to developing statistical mechanics, seeking to explain macroscopic laws such as temperature and entropy through the invisible motion of atoms. At the time, even the existence of atoms was widely questioned, and his ideas faced strong resistance. Boltzmann spent decades refining and defending his theory, often working in isolation as he struggled with the gap between mathematical insight and experimental acceptance. Although his contributions were not fully recognized during his lifetime, they later became foundational to modern physics. His story reminds us that deep understanding often demands patience measured in years—or even lifetimes—and that the intrinsic story of nature may take a long time to align with human belief.

Through my (young) experience as researcher, I also have learned that mental well-being is closely tied to the research process. The research can start to feel routine when the curiosity fade, and when pressure builds, even small setbacks can seem overwhelming. What has helped me most is accepting uncertainty as a natural part of research rather than something to be avoided. In surface science, imperfections such as defects are often what make a surface more active and interesting. In the same way, research rarely advances through perfectly smooth paths; it progresses unevenly, shaped by unexpected results and exploration rather than perfect/expected results.

Human connection is just as important in the research journey. Conversations with colleagues, especially between experimentalists and theorists, often lead to deeper understanding than working alone. Explaining an idea helps clarify thinking, while listening to others can reveal assumptions one might not notice. In these moments, research becomes a shared human effort, built through dialogue and learning together.

This interaction can be seen clearly in the relationship between experiment and theory. Experiments show how nature behaves in real conditions, while theory helps explain those observations. Neither works well on its own. Without theory, experimental results are hard to understand, and without experiment, theory cannot be tested. Progress happens when the two continue to inform each other. This concept has actually shaped how I view research: not as a one-directional process, but as an ongoing conversation. As long as this dialogue continues, research remains not only a means of discovery, but a profoundly human endeavor.

As a closing to this article, I would like to share a message with fellow young researchers (and as a reminder for me too). It is natural to feel discouraged when progress is slow or when results do not turn out as expected. Research, like any good story, rarely unfolds in a straight line; uncertainty, detours, and unanswered questions are part of the narrative. By staying curious and patient, and by continuing to engage with both the story written by nature and the story we build through our own efforts, research can remain meaningful and rewarding. I hope that, together, our generation can contribute to a beautiful scientific story—one that will be remembered and built upon in the future.