Imperagen

Chemistry Will Become Programmable

A Manifesto for Large Reaction Models

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AI is crossing domains

AI's first great public breakthrough was language. **Large Language Models** absorbed a meaningful share of human knowledge and gave us a new way to work with it. We could ask, challenge, create and reason through conversation. Knowledge became something we could talk to.

Now AI is crossing into the physical world. **Large World Models** are learning from video, sensors and action. They are beginning to understand that objects have weight, motion has consequences and a robot reaching for a cup either grasps it or misses. Reality answers back.

There is another physical world beneath anything a camera can see.

At the molecular scale, proteins flex, atoms move, electrons shift and bonds form or break. These tiny events decide whether a medicine can be made, a material will degrade, a crop can be protected or a biological system keeps working. The molecular world builds the visible one.

Large Language Models learned patterns across human knowledge. Large World Models are learning physical cause and effect. We believe reaction space will become the next great domain for AI.

The models built to learn it will be **Large Reaction Models**.

Chemistry will become programmable.

The world beneath the world

Chemistry is how humanity turns matter into value. It gives us antibiotics and semiconductors, fertilizers and batteries, clean water and modern materials. Almost everything we make depends on our ability to turn one form of matter into another.

Yet chemistry remains stubbornly difficult. A useful reaction may depend on a fleeting movement, a tiny energy difference or a condition that nobody thought to test. Progress still relies on exceptional people, long campaigns and a great deal of trial and error. Hard-earned knowledge is scattered across papers, patents, notebooks and the memories of scientists.

The cost is measured in years, capital, wasted material and ideas that never leave the lab.

We can do better.

The molecular world is waiting for AI to learn it.

From molecular form to molecular action

AlphaFold showed what happens when AI enters a scientific field at scale. Protein structure, one of biology's deepest problems, became computable with an accuracy few believed possible. Generative models are already designing new proteins and exploring structures nature never found.

Those breakthroughs gave us extraordinary maps of molecular form.

The next frontier is what happens on those maps.

How does a protein behave when it meets a molecule? Which path will a reaction take? What change will make it faster, cleaner or more selective? Could a biological catalyst perform chemistry that nature never needed? Could an entirely new route appear?

Large Reaction Models are the intelligence layer for those questions. They will learn across proteins, molecules, motion, energy, experimental results and the conditions that shape a reaction. They will help scientists move through reaction space with purpose.

A desired outcome could become the starting point. From there, the model would find credible routes, propose catalysts, learn from what happens and keep moving.

Over time, the map becomes a guide and then an engine for discovery.

Closing the innermost loop

AI becomes far more powerful when it can act, observe and learn again. Chemistry has struggled to build that loop because molecules still get the final vote. The system needs a way to touch reality.

High-throughput automated laboratories are changing that. They allow AI to propose experiments, test them in molecular reality, learn from the results and decide what to try next. The wet lab becomes the model's sensor into the molecular world. This loop is what makes Large Reaction Models possible now.

This is the recursive self-learning AI path into the molecular world.

The unimaginable becomes inevitable

Once chemistry becomes programmable, entirely new horizons open.

New medicines can be made through shorter, cleaner routes. Innovative materials can be designed around the properties we want, instead of the feedstocks and processes we inherited. Stubborn waste can become raw material. New products emerge using much less energy and creating significantly less pollution.

Enzymes are the natural starting point. They already make, modify, copy, break down and repair molecules throughout nature. With far better reaction intelligence, we can push them into work evolution never selected for: manufacturing a complex drug, synthesizing DNA and RNA on demand, protecting crops with minimal environmental damage, replacing harsh industrial processes, removing persistent pollutants, or even reversing aspects of aging, one molecular repair at a time.

Some of these possibilities sound audacious today. So did speaking naturally with a machine. So did predicting the structure of almost every known protein. Much of what now feels inevitable once sounded unimaginable. The shift can happen remarkably fast.

A new interface to matter

Imagine beginning with the outcome you want.

Make the molecule at the heart of a new medicine targeting a previously unreachable pathway. Create a polymer that performs brilliantly and then safely disappears. Turn this waste stream into something valuable. Repair this damaged molecule in our skin or eyes. Find a biological route to a material that does not exist yet.

This new intelligence system would search possibilities no person could hold in mind, learn from the world's scientific knowledge and then test its best ideas against reality. Each experiment would deepen the model. Each new problem would begin with more intelligence than the one before it.

The change would reach far beyond faster research.

When chemistry becomes programmable, invention itself changes. More people can begin with the outcome they need, rather than the chemistry they already know. The distance between imagination and physical creation begins to collapse.

Matter becomes a medium we can work with far more freely.

Every great industrial age has been shaped by a new command of matter. Bronze. Steel. Petrochemicals. Silicon. Each opened possibilities that the generation before could barely imagine.

Reaction intelligence will open the next one.

Today, invention is constrained by the reactions we already know and the processes we can afford to run. In a programmable molecular world, we can begin somewhere more human: with what we need.

Medicines that reach people faster. Materials that perform without poisoning the planet. Food produced with fewer resources. Manufacturing that works with biology instead of fighting it. New ways to protect, restore and extend healthy life.

Then we ask chemistry to find a way.

Human imagination has always run ahead of our ability to make. Large Reaction Models can begin to close that distance.

The prize

The molecular economy is measured in trillions of dollars, but its true value is everywhere: in health, food, energy, climate, materials and the resilience of the systems people depend on.

We learned to use code to command electrons, and the digital world followed. Learning to navigate reaction space could give us a new interface to matter itself.

This intelligence will grow through use. Every experiment adds to what the model understands. Better understanding leads to better questions, better experiments and more ambitious problems coming within reach.

At **Imperagen**, enzymes are our path into this future. They are nature's molecular machines, and they give us a powerful place to begin. Our ambition reaches much further: to build Large Reaction Models that learn from the molecular world and help humanity shape it.

What we believe

We believe AI's journey from language into the physical world will continue into the molecular world.

We believe reaction space is one of the largest and most valuable domains left to learn.

We believe automated wet labs will give AI a sensor into molecular reality, turning recursive experiments into compounding intelligence.

We believe enzymes can be pushed far beyond the functions nature happened to select.

We believe cleaner manufacturing, new materials, programmable biology and molecular repair belong to the same expanding frontier.

We believe some of the hardest problems in health, industry and the environment will become reaction problems we can solve.

We believe chemistry will become programmable.

That is the future we are building.