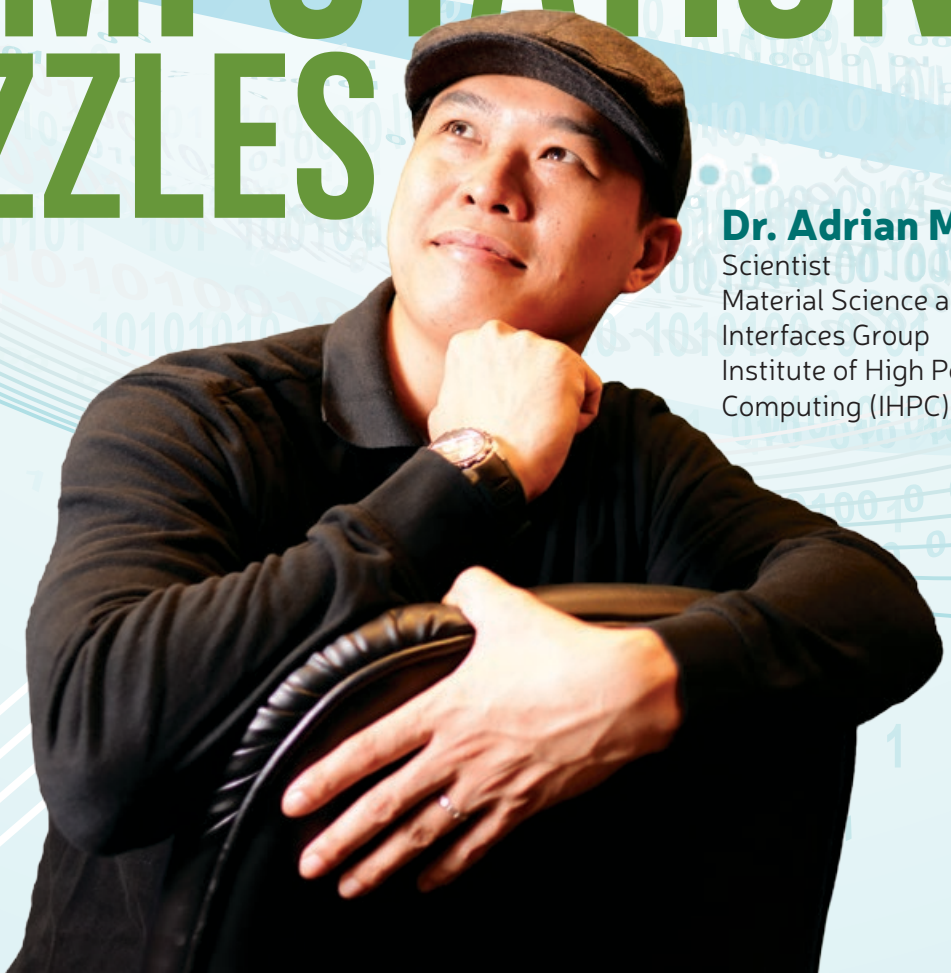
DECIPHERING COMPUTATIONAL PUZZLES

Schrödinger's equation, multipole moments, Hartree-Fock approximation and other tongue-twisting terms are likely to pop up if you get scientist Adrian Matthew Mak to talk about what he does. But most of the time, he gets off the hook by telling people that he models and simulates chemicals on very powerful computers. "They are usually intrigued by the 'powerful computers bit'," quips Adrian.

What with the Nobel Prize in Chemistry going to computational chemists Martin Karplus, Michael Levitt, and Arieh Warshel last year, this is a field that is fast gaining much attention these days. It is the stuff brainiacs dream of – computational chemistry integrates the knowledge from multiple disciplines such as physics, chemistry, mathematics, computer science and engineering, and harnesses high performance computing to help answer diverse problems.

Cracking Real-world Puzzles

Solving tough puzzles is what draws Adrian. The scientist, who is a cruciverbalist – someone who cracks crossword puzzles for fun – is immensely interested in finding new methods in electronic structure. "How matter behaves is governed by different rules on different scales. At the very small scale, properties of molecules are dictated by electrons and nuclei, and their behaviour is in turn governed by the rules of quantum mechanics," explains Adrian. "So I work on novel methods to better describe the behaviour of electrons, and implement these methods in software packages for computers to calculate and predict the behaviour of atoms and molecules."



Dr. Adrian Matthew Mak
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If this makes him sound like an armchair, mouse-clicking theoretician, it is actually quite off the mark. Over the years at A*STAR, Adrian has also worked on a huge range of projects with real-life applications, from designing catalysts for specialty chemicals to simulating materials for electronics.

"I do treasure my armchair moments, but real-world problems can drive the advance of theoretical knowledge," Adrian shares. "For example, when you look at a complicated chemical reaction happening in a flask, you can't really tell much just by staring at it. Computational chemical models can help us achieve better understanding of the processes that take place. And in the case of developing new materials for various purposes, by combining the art of computational chemistry and materials science, coupled with powerful computers and software, we can model and simulate these materials and predict how they will behave even before they are made. This helps to save time and resources."

Gone are the days when scientists hole up and shut themselves in the laboratory all day. When it comes to finding answers to the complex questions scientists face today, the process is now highly collaborative. It is a diverse community that Adrian finds himself working in – one where engineers, chemists, biologists and physicists come together, each bringing a piece of the puzzle to form a clearer, bigger picture of the problem and the solution.

"A career in science provides the intellectual challenge that is intrinsically rewarding to me."

No Scientist Is An Island

The impact of Adrian's work clearly goes beyond his laboratory. "We work with other research institutes, local and overseas universities and the industry," Adrian says. "Personally, I find computational chemistry to be very useful to my colleagues in other A*STAR's research institutes. The modelling and simulation results help to explain their experimental observations, and guide them in the design and synthesis of new chemicals and materials for different uses."

Breaking Boundaries

As a child, Adrian had dreamt of becoming a fighter pilot, a doctor, a teacher and an astronaut. Today, his work in computational chemistry is a happy blend of all the things he loves – the elements, numbers, and computers.

When opportunities arise, Adrian would share his passion for science with others through platforms such as lectures and school talks. Says the chemist, "We need young people who have a thirst for creating new things, modifying what's on the shelf, and inventing "life hacks". We need to challenge status quo, try new things, break new territory and not be afraid of taking on measured risks while experimenting with the tools we use for work and play."

These qualities are exactly the same ones that drive him. "Unlike many other jobs, a career in science provides the intellectual challenge that is intrinsically rewarding to me," Adrian asserts. "I stand on the shoulders of giants to contribute what I can to the bag of tricks used in computational chemistry methods, and to science in general. When I have an epiphany, and I start to go, 'Hey, I think I know why things work this way,' or 'I think I can prove this conjecture of mine'". These are the little victories that make my day, and add meaning to what I do."