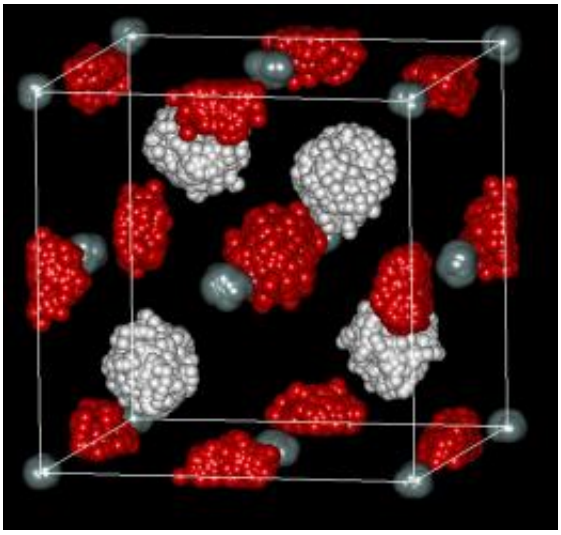
Unveiling the behavior of hydrogen molecules

May 6 2011



Dr. William Yim had the opportunity to collaborate with Toshiaki Iitaka from Riken Advanced Science Institute and Prof John Tse from Canada's University of Saskatchewan last year. The team of researchers discovered the physical basis to explain the newly discovered vibration behavior of molecular hydrogen, including 'silane' - hydrogen bound to silicon, under high pressure.

The two-month project resulted in a paper, 'Pressure-induced intermolecular interactions in crystalline silane-hydrogen', that was published in *Physical Review Letters* 105.

The cross-disciplinary team was like a dream team, made possible by the mutual introductions given by Prof John Tse and Dr. Wu Ping, IHPC's Director of Material Science and Engineering Department.

"Prof. John Tse's expertise is on experimental and computational research on materials science and he is famous in high pressure research field" said William. "Dr. Toshiaski Iitaka is a permanent staff member at Riken working on solid state research and program development for linear scaling computational method."

As William himself has a track record on ab initio vibrational frequency calculations applying to surface science, it was a good match of expertise.

His motto is "Be Prepared", so the challenge of taking on the project was a welcome one.

"I like to learn new skills, and I made sure I learnt all the necessary computational techniques before this project. Good preparation and speed are the key factors in benefitting from such a good opportunity."

It was a classic collaboration case study, in which everyone played an important role in making the breakthrough.

"When Prof. Tse mentioned an interesting problem of H2 vibron softening, we were well prepared to puzzle out the scientific question" William said.

William contributed the 'Donor-acceptor interaction in compression regime', which is a brand new idea.

The team performed molecular dynamic simulations to study the interactions between hydrogen and silane molecules, which gave a better

fundamental understanding for the materials under extreme conditions.

The results provided a good basis to potentially develop a hydrogen economy.

William said “the knowledge of physical interaction in compressed regimes, as indicated by vibrational spectroscopy and chemical bonding, will be very helpful for further engineering the mixing process and hence the H2 transport capability.”

The project is another feather in the cap for IHPC.

Dr. Toshiaki Itaka, from Riken’s Computational Astrophysics Laboratory commented: “It was an exciting experience that I could work with William and IHPC for the study of SiH4 under pressure. As a physicist, I learned a lot from the chemist's viewpoint of William.”

“I also noted that IHPC has strength not only in academic research but also in its application to important problems in real world. This is what Riken is aiming at, and would like to learn from IHPC.”

William too had an enriching experience working closely with the other researchers, commenting “the most important skill I’ve learnt is to understand how to translate research work into an impactful and engaging story. It is an art to turn lots of boring numbers into an interesting story so that people can understand the significance of the discovery.”

Provided by Institute of High Performance Computing, Singapore