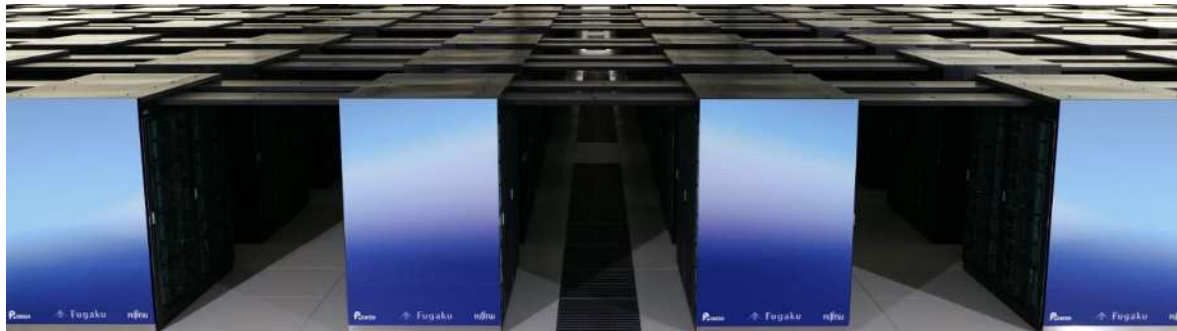
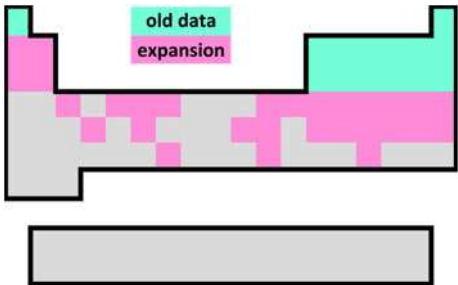


Name CHAN Bun	Job Title Associate Professor	Area of Expertise Quantum Mechanics, Computational Chemistry, Chemical Data Science
1. Main Research Topic  Our research involves the use of high-performance computers for quantum chemistry. We develop new methods to accelerate the simulations, to model a wide range of chemical and materials systems. Such modellings are often conducted in collaboration with experimentalists, providing knowledge at the electronic level to develop new technologies. Below you will find a few examples of our work. (1) High-precision quantum chemistry methods are traditionally applicable only to a limited range of chemicals, covering a small portion of the periodic table. We have developed a series of quantum chemistry methods to expand the scope of high-precision prediction, to provide reliable data for machine learning in chemistry. - Chan, B. Accurate Thermochemistry for Main-Group Elements up to Xenon with the Wn-P34 Series of Composite Methods. <i>J. Chem. Theory Comput.</i> 2021, 17, 5704. - Chan, B. Compilation of Ionic Clusters with the Rock Salt Structure: Accurate Benchmark Thermochemical Data, Assessment of Quantum Chemistry Methods, and the Convergence Behavior of Lattice Energies. <i>J. Phys. Chem. A</i> 2023, 127, 5652.  (2) In a collaboration with several international research teams, we apply quantum chemistry to clarify structural features that leads to luminesce in a new type of glass materials. - Hou, J.; Chen, P.; Shukla, A.; Krajnc, A.; Wang, T.; Li, X.; Doasa, R.; Tizei, L. H. G.; Chan, B.; Johnstone, D. N. et al. Liquid-Phase Sintering of Lead Halide Perovskites and Metal-Organic Framework Glasses. <i>Science</i> 2021, 374, 621.		
2. Keywords Quantum chemistry Chemical physics Molecular biology Materials science Chemical data science		
3. Remarks and Website researchmap: https://researchmap.jp/el_buno Laboratory: https://sites.google.com/view/bunchan Google scholar: https://scholar.google.com/citations?user=URuEgEoAAAAJ&hl=en		