Supercomputer-rescued quantum chemical modeling

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Quantum chemical modeling is widely used throughout the chemical sciences. It is particularly important in the fields of biochemistry and molecular catalysis. The most commonly used quantum chemical method is the Density Functional Theory (DFT), which can correctly describe bonds cleavage and formation, and has an optimum cost-to-accuracy ratio. To obtain correct results from DFT calculation, one should carefully choose both functional and system model.

The talk will consider the problems of choosing adequate functional[1,2], system model[3] and other modeling parameters. Also, several examples of practical modelings[4–6] will be discussed and the overall necessity of applying supercomputers to the real-world chemical problems will be demonstrated.

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