Progress of adaptive finite element (FE) method in solving nonlinear partial differential equation (PDE)

Scientific computation is widely used in multiple cross-disciplinary areas. Most of the issues coming from this area finally result in solving PDE. In the process of solving PDE, the meshes are firstly generated within the area where PDE is functional; then, the methods of FE, Finite Difference (FD), and Finite Volume (FV) are applied on the meshes to solve the PDE. Because of the unknown results of the PDE, the traditional methods for the mesh generation are experiential. This strategy mostly results in the low efficiency in the complicated engineering computing environment especially for those nonlinear problems, and confines the application scope of these discretized methods.

Adaptive Finite Element (AFE) method is a discretized method that automatically coordinates the finite element mesh to optimize the computation complexity according to the convergent accuracy of the results and the characteristics of the solutions. This method is based on the theory of posteriori error analysis, can be widely used and programmed by software, and becomes one of the focuses of scientific computation. With the consistent support from NSFC, especially the support from the fund for National Distinguished Young Scholars, Prof. Zhiming Chen from Academy of Mathematics and Systems Science, CAS, progressed in their research in the nonlinear problems of posteriori error analysis and adaptivity in the topics of elliptical calculus of variations, superconductivity, continuous casting, electromagnetic scattering and the Richards equation for the mobility of non-saturated water:

1. The scientific computation on the unconfined area for electromagnetic scattering became an important subject with extensive considerations. The global research focused on the trace to solve electromagnetic scattering problems casting on the technique of the perfectly matched layer (PML), which was firstly proposed in 1994 using FE method. Prof. Chen and his research team further developed and published Adaptive PML for grating problems and 2D acoustic scattering problems, namely, utilized the theory of posteriori error analysis to define the parameters of PML. They overcame the deficiency from experientially defined parameters in engineering computation. And this method possesses prosperous application future and theoretical significance.

2. Nonlinear conductive-diffusive equation is widely utilized in the scientific computation of fluid mechanics. Prof. Chen obtained new results, which could not be solved by traditional numerical methods, in allusion to nonlinear Richards' equations for the mobility of non-saturated water, by applying the famous Kruzkov method of posteriori error analysis in nonlinear balance equation to nonlinear parabolic equation with boundary conditions. Prof. Chen further improved their AFE method with *Method of Line* (AML) to solve the nonlinear conductive-diffusive equation based on the previous approach. A majority computation results showed that this new improved algorithm had the optimized computation complexity for evolutionary problems. Although the fact that AFE method had the optimized computation complexity for the elliptic problems, for the evolutionary problems, AML was not recognized and deeply studied in its optimized computation complexity before Prof. Chen's work. Prof. Chen's innovation clarified that AML method of parabolic equation had better optimized computation complexity than AFE.

Prof. Chen gained praising evaluation from international colleagues on the innovative research of AFE, and was invited to present a 45-min lecture on the 2006 International Congress of Mathematicians held in Spain.

Controlling the electromagnetism of single ion by "molecular surgery"

Controlling and modifying the magnetic property of a single molecule is the frontier for the development of molecular science. With the funding support from NSFC, Scientific Innovation Program of CAS as well as 973 from Ministry of Science and Technology of China, Prof. Jianguo Hou (Member of CAS) and Prof. Jinlong Yang from National Laboratory for Physical Sciences at the Microscale of University of Science & Technology of China, together with Prof. Qingshi Zhu (Member of CAS), made an artifice surgical operation to a single CoPc molecule that attached on a metal surface with facility of Scanning Tunneling Microscopy (STM), and achieved to control the spin state of a single molecule. They published this achievement as a report on Science magazine on Sep. 2, 2005.

In their experiment, they scattered and deposited a small amount of CoPc molecules on clean Au surface through evaporation process, and systematically studied the surface physical and chemical properties of this molecule by STM. They found that, once landed on the Au surface, the magnetic property of CoPc molecule quenched in the reaction between the molecule and the metal surface. Since the outside of the coordinated compound of CoPc molecule is formed by 4 Benzene rings, 8 periphery hydrogen atoms of those Benzene rings could be pruned off from the molecule to activate C-H bonds on these Benzene rings by tunnel electron with a specific power provided by STM tip. After this surgery, stable chemical bonds were formed between Benzene-ring radicals without hydrogen atoms and Au surface, and then, the structure of the artificial molecule was established. They also found that, the Scanning Tunneling Spectroscopy (STS) of ion Co, which was in the middle of this artificial molecule structure, displayed Kondo effect induced by local magnetic dirt, namely, the original resonance with the large half-width on the hybridized d-level was substituted by a sharp resonance near Fermi surface. It was indicated by shape, width, and their temperature dependent varieties that the effect was Kondo effect. This phenomenon proved that ion Co of CoPc, which lost its hydrogen atoms, possessed a local magnetic torque; so, the magnetic property of the molecule was recovered. The localized spin within the structure of the artificial molecule was proved by theoretical computation and analysis based on First-Principles. The experimental results reappeared when the theoretical simulation of STM images were implemented.

This research achievement displayed how to manipulate chemical reactions within a single compound molecule, then, adjust and control the spin state of magnetic metal ion within a molecule. Furthermore, the research developed an important new method to make the functional units of a single molecule, and disclosed the extensive prosperous future for the research in molecular science. In the Perspective session of Science magazine (Sep. 2, 2005), Prof. Michael F. Crommie wrote a report, titled *Manipulating Magnetism in a Single Molecule*, to describe and praise this research achievement. In the report, he wrote "The result opens the way for fundamental studies

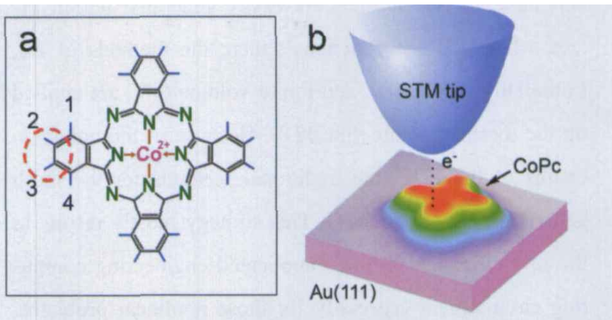

Fig. 1(a) Molecular structure of cobalt phthalocyanine: 4 benzene rings outside, 2 or 3 hydrogen atoms would be removed from the ring. (b) Hydrogen atoms of cobalt phthalocyanine were activated by a specific power by STM tip and were pruned off by tunneling electrons.

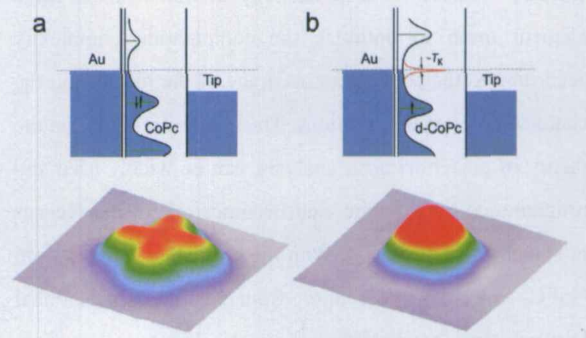

Fig. 2(a) Cobalt phthalocyanine molecule (bottom part) was attached on the metal surface. There is only a resonance with the large half-width on the hybridized d-level near Fermi surface on the STS of central Co Ion (top part). (b) The artificial molecular structure without hydrogen atoms (bottom part). There was a sharp resonance stably attached on Fermi surface. This displayed the localized magnetic torque (top part).

of spin behavior in molecules that may influence future molecular device applications".

Progress in synthesizing functional nano materials

With the consistent investment, the research team directed by Prof. Yadong Li of Chemistry Department of Tsinghua University achieved new progress in synthesizing nano materials with specific functions. The research team led by Prof. Li devoted their efforts in the research of