综合报告会

Lecture

国家数学与交叉科学中心

Time: 10:20 am, September 16
Venue: S712

The mathematics of quantum molecular simulation

Speaker: Prof. Eric Cances

Ecole des Ponts- ParisTech and INRIA, France

Abstract :
Quantum molecular simulation has become a major tool in chemistry, condensed matter physics, materials science, molecular biology and nanotechnology. It is also an inexhaustible source of exciting mathematical and numerical issues. This lecture aims at giving an overview of the models used in quantum molecular simulation, with a special focus on density functional theory (DFT), and at presenting some recent advances and open questions on the mathematical and numerical analysis of these models.

Brief CV:
Eric Cances is a Professor of Applied Mathematics at Ecole des Ponts and Ecole Polytechnique in Paris. He is also a member of the INRIA project Micmac. His research interests focus on the mathematical and numerical analysis of molecular and multiscale models, with applications in chemistry and materials sciences. He is co-author of two books and about 50 research articles. In 2009, he was awarded the Blaise Pascal prize from the French Academy of Sciences.