Oberwolfach Seminar: The Mathematics of Quantum Chemistry

Date: November 24 – November 30, 2013

Organisers:

Eric Cancès, Paris
Gero Friesecke, München
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Programme:

Quantum mechanics is the key to any deeper understanding of the behavior of atomic and molecular systems. Quantum mechanical calculations are central to modeling molecular processes with applications in chemistry, biochemistry, solid state physics, and nano-sciences. In mathematical terms, the basic problem is to find the solutions of the Schrödinger equation for a system of electrons and atomic nuclei that interact by electrostatic attraction and repulsion forces. Due to the high-dimensionality of the problem, approximating the solutions is inordinately challenging and not possible with the standard methods of numerical mathematics. Despite tremendous progress within the last decades and a deep impact in sciences and technology, the field of quantum mechanical calculations has been rather ignored in numerical analysis and applied mathematics. This unsatisfying situation is presently changing. The purpose of this seminar is to give an introduction to this field and its mathematical background and the challenges that it constitutes for analysis and numerical mathematics. It is intended to make the seminar accessible to participants with no or only minor background in physics and chemistry.

Preparatory reading:

Le Bris, C.: Computational chemistry from the perspective of numerical analysis. Acta Numerica 14, 363–444 (2005)

Helgaker, T., Jørgensen, P., Olsen, J.: Molecular Electronic Structure Theory. John Wiley & Sons, Chichester (2000)