Thursday, Jan 25, at 16:00-17:00

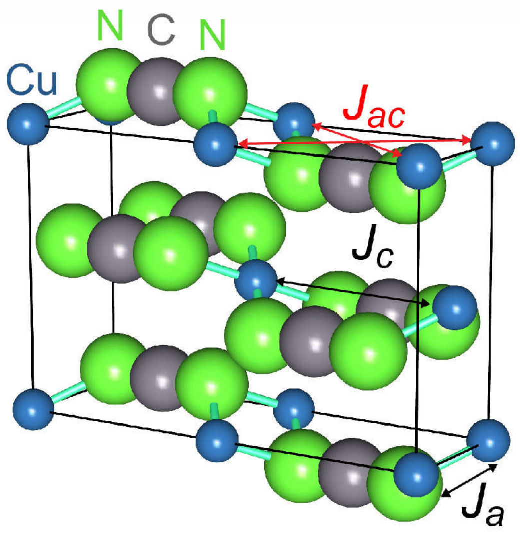
Skoltech, Blue Bldg, room 402

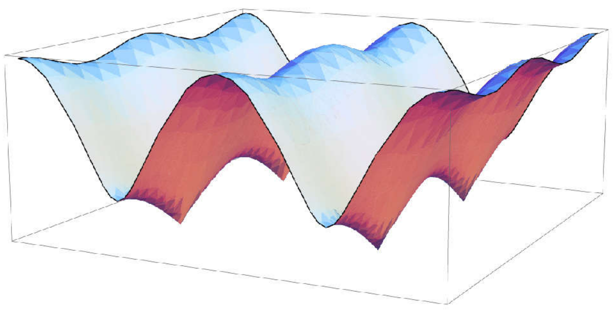
Skoltech

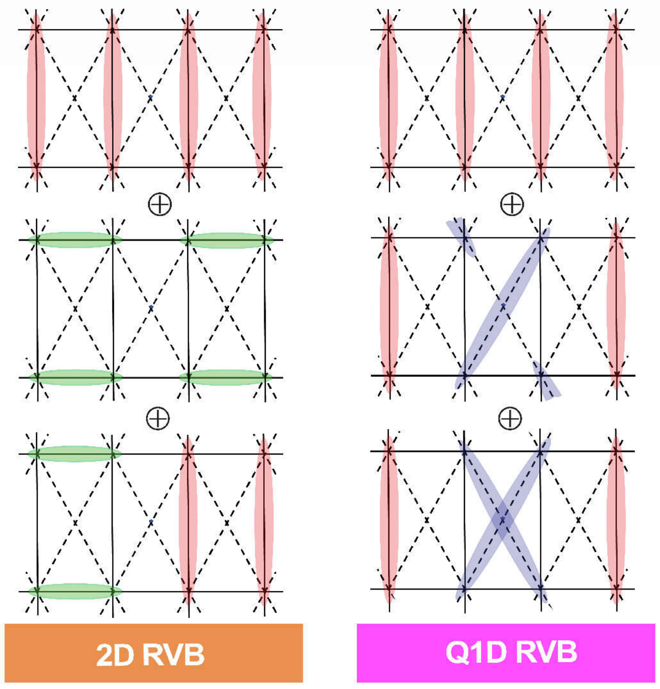
Skolkovo Institute of Science and Technology

Resonating Valence Bonds:

A Lost Tribe of Solid-State Quantum Chemistry







Speaker

Andrei L. Tchougréeff[1,2,3]

[1] *Institute of Inorganic Chemistry, RWTH - Aachen University, Germany*

[2] *Independent University of Moscow, Russia*

[3] *A.N. Frumkin Institute of Physical Chemistry & Electrochemistry of RAS, Russia*

Abstract:

The concept of (chemical) bonding is widely spread, but it is rarely realized that in fact it is based on very archetypical features of human thinking which may manifest in very different formal disguises remaining substantially unchanged. In the first part of this talk I am going to give some kind of historical perspective of the genesis of the idea of chemical bond and demonstrate how this concept may be (and actually had been many times) used for developing quantum chemistry methods explicitly employing the idea of bonding. Next, the limitations of the concept of the isolated chemical bond well known in (quantum) chemistry will be highlighted and two recipes known to handle these restrictions will be confronted (molecular orbitals - MO vs (resonating) valence bonds - (R)VB). Finally, the implications of the RVB hypothesis for a specific solid state problem (CuNCN physics) will be presented.

Very remarkably, the RVB states cannot be reproduced by any available solid state quantum chemistry software which is absolutely and alternativelessly dominated by the Hartree-Fock approximation. The very possibility of the RVB ground state is not programmed, which makes it elusive due to this restriction of the software. The situation is in a way scandalous in a view of importance of the RVB states for the high-Tc behavior, but also due to its possible wider occurrence in practice as proven by our CuNCN experience.

Biography:

Andrei L. Tchougréeff graduated in 1982 from the Lomonosov Moscow State University. In 1989 he obtained Ph.D. from the Karpov Institute. In 2004, Dr. Tchougréeff earned the title of Doctor habilitated from the Karpov Institute. During this period he conducted theoretical and computational studies of electronic structure of complex molecular systems. From 2008, Dr. Tchougréeff is a leading scientist at the Institut für Anorganische Chemie der Rheinisch-Westfälischen Technischen Hochschule (RWTH Aachen University) and from 2017 at the Frumkin Institute of Physical Chemistry and Electrochemistry of Russian Academy of Science. The fields of his research include theoretical solid state inorganic chemistry (carbodiimides, spin-active transition metal complexes and crystals, magnetic interactions), quantum chemistry (correlated systems, complex systems, O(N) scalability from physical grounds, low-dimensional systems, resonating valence bonds, catalysis by transition metal complexes), and analytical solutions in theoretical chemistry.

Looking forward to seeing you!