Report-2017, M.-Corr. Boris Tsukerblat

Papers

1. B. Tsukerblat, A. Palii, J. M. Clemente-Juan, E. Coronado, Jahn-Teller effect in molecular electronics: quantum cellular automata, *Journal of Physics: Conference Series,* 833 (2017) 012002

2. S.M. Aldoshin, D.V. Korchagin, A. V. Palii, **B.S. Tsukerblat**, Some new trends in the design of single molecule magnets, *Pure and Applied Chemistry*, 89 (2017) 1119-1143.

3. M. Nazarov, M.G. Brik, D. Spassky, **B. Tsukerblat**, Crystal field splitting of 5d states and luminescence mechanism in $SrAl_2O_4:Eu^{2+}$ Phosphor, *J. Luminescence* 182 (2017) 79–86.

4. A. Palii, S. Aldoshin, **B. Tsukerblat**, J. M. Clemente-Juan, A.Gaita-Ariño, E. Coronado, Electric field controllable magnetic coupling of localized spins mediated by itinerant electron: a toy model, *Physical Chemistry Chemical Physics*, 19 (2017) 26098-26106.

5. A. Palii, S. Aldoshin, **B. Tsukerblat,** J. J. Borràs-Almenar, J. M. Clemente-Juan, S.Cardona-Serra, E.Coronado, Electric field generation and control of bipartite quantum entanglement between electronic spins in mixed-valence polyoxovanadate $[GeV_{14}O_{40}]^{8-}$, *Inorganic Chemistry,* 56 (2017)9547-9554.

6. D. V. Korchagin, A. V. Palii, E. A. Yureva, A.V. Akimov, E.Ya. Misochko, G.V. Shilov, A.D. Talantsev, R.B. Morgunov, A.A. Shakin, S. M. Aldoshin, **B.S. Tsukerblat**, Evidence of field induced slow magnetic relaxation in cis-$[Co(hfac)_2(H_2O)_2]$ exhibiting tri-axial anisotropy with a negative axial component, *Dalton Transactions*, 46 (2017) 7540-7548.

7. A. Palii, S. Aldoshin, **B. Tsukerblat**, Mixed-valence triferrocenium complex with electric field controllable superexchange as a molecular implementation of triple quantum dot, *Journal of Physical Chemistry C* 121, 2017, 27218−27224.

8. S. M. Aldoshin, A.V. Palii, D.V. Korchagin, **B.S. Tsukerblat**, New magnetic materials based on single molecule magnets, *Proceedings of the Sixteen Bi-national Workshop Russia-Israel*, 2017, pp. 255-278.

9. A. Palii, S. Aldoshin, **B. Tsukerblat**, J. M. Clemente-Juan, A. Gaita-Ariño, E. Coronado, Electric field control of molecular magnetic switching, *Proceedings of the Sixteen Bi-national Workshop Russia-Israel*, 2017, pp. 279-290.

10. B. Tsukerblat, A. Palii, J.M. Clemente-Juan, N. Suaud, E. Coronado, Quantum cellular automata: a short overview of molecular problem, *Acta Physica Polonica* A (in press).

11. J.M. Clemente-Juan, A. Palii, **B. Tsukerblat**, E.Coronado, VIBPACK: A Package to treat multidimensional electron-vibrational molecular problems with application to magnetic and optical properties, *J. Comp. Chemistry* (in press).

12. B. Tsukerblat, A. Tarantul, A. Palii, S. Aldoshin, An unique nanoscopic polyoxometalate V_{15} : exchange coupling and magnetic anisotropy, *J. Coord. Chemistry* (submitted).

International Conferences

1. **B. Tsukerblat,** A. Palii, J.M. Clemente-Juan, E. Coronado, N. Suaud , A paradigm of quantum cellular automata: implementation of molecular magnets, 15th European Conference Physics of Magnetism 2017 (PM'17), Poznań (Poland), June 26-30, 2017 (plenary, invited).
2. A. Palii, S. Aldoshin, **B. Tsukerblat**, J.M. Clemente-Juan, E. Coronado, Electric field controllable bipartite quantum entalgnement in mixed-valence polyoxovanadate $[VGe_4O_{40}]^{8-}$, XI Russian-Japanese workshop "*Open shell compounds and molecular spin devices*", Japan, 12-15 November, 2017 (invited).
3. A.Palii, S. Aldoshin, **B. Tsukerblat**, J.M. Clemente-Juan, A. Gaita-Ariño, E. Coronado, Electric field control of molecular magnetic switching, The 16th Israeli - Russian Bi-National Workshop 2017, "*The optimization of composition, structure and properties of metals, oxides , oxides, composites, nano and amorphous materials*" , 28-31 July, Ariel, Israel (invited).
4. S.M. Aldoshin, A.V. Palii, D.V. Korchagin, **B.S. Tsukerblat**, New magnetic materials based on single molecule magnets, The 16th Israeli - Russian Bi-National Workshop 2017, "*The optimization of composition, structure and properties of metals, oxides , oxides, composites, nano and amorphous materials*", 28-31 July, Ariel, Israel (plenary, invited).

The main results:

1. We have proposed a toy model to describe the magnetic coupling between the localized spins mediated by the itinerant electron in partially delocalized mixed-valence systems. The proposed descriptive model is exactly solvable that allowed us to qualitatively and quantitatively discuss the main features of whole class of the partially delocalized systems. In the case of relatively strong exchange coupling the combined action of these two interactions is shown to give rise to a specific kind of double exchange coupling termed here "external core" double exchange. In the opposite case of a relatively strong electron transfer the general Hamiltonian is shown to be reduced to the effective Hamiltonian of indirect exchange for the localized spins. We argue a possibility to efficiently control the magnetic coupling of the localized spins by an external electric field acting on the delocalized part of the system.

2. We have developed a computational approach (including a FORTRAN code) based on a to solve multidimensional dynamic Jahn-Teller and pseudo Jahn-Teller problems. This symmetry-assisted approach constituting a theoretical core of the program is based on the full

exploration of the point symmetry of the electronic and vibrational states. We also reported some selected examples of increasing complexity aimed to display the theoretical background as well as the advantages and capabilities of the program to evaluate of the energy pattern, magnetic and optical properties of large multimode vibronic systems.

3. In quest of the systems in which control of quantum entanglement can be achieved, here we consider the paramagnetic mixed-valence polyoxometalate $K_2Na_6[GeV_{14}O_{40}]\cdot 10H_2O$. Applying a homogeneous electric field one can induce antiferromagnetic coupling between the two delocalized electronic spins which behave as independent in the absence of the field. Based the developed theoretical model we show that as a consequence, the external field can be used to generate controllable quantum entanglement between the two electronic spins travelling over vanadium network of mixed-valence polyoxoanion $[GeV_{14}O_{40}]^{8-}$. Within a simplified two-level picture of the electronic pair based on the previous *ab initio* analysis we evaluate the temperature and field dependences of concurrence and thus indicate that the entanglement can be controlled via temperature, magnitude and orientation of the electric field with respect to molecular axes.

4. We made a combined experimental characterization and theoretical modeling of the hexa-coordinated high-spin Co(II) complex *cis*-$[Co(hfac)_2(H_2O)_2]$. The magnetic DC data and EPR spectra were analyzed with the aid of the Griffith Hamiltonian supported by the ab initio calculations of the crystal field parameters, *g*-factors and superexchange parameters between H-bonded Co(II) ions. This analysis suggests the presence of the easy axis of magnetic anisotropy and also shows the existence of a significant rhombic component. Frequency dependent susceptibility signal shows that the complex exhibits slow paramagnetic relaxation in applied DC field belonging thus to the class of non-uniaxial field induced single ion magnets with negative axial anisotropy. The main contributions to the relaxation come from the direct one-phonon process dominating at low temperatures, while the contribution of the two-phonon Raman process becomes important with increasing temperature.

5. We proposed molecular implementation of the quantum logic gate originally realized by the linear triple-quantum dot array accommodating two electrons. To reach this goal we propose to employ the mixed-valence triferrocenium complex. The interaction of the electrons with the applied electric field is also included in the Hamiltonian. It is shown that due to long-range superexchange between the two electronic spins the ground state of trierrocenium complex is always a spin-singlet and the first excited level is a spin-triplet. The electric field is

shown to increase the antiferromagnetic exchange coupling. Estimations of the efficiency of the electric field control of the exchange coupling and entanglement show that the triferrocenium complex is emerging as potential candidate to act as a gate in quantum computing.