RAS Scientific Council on chemical kinetics and structure
Division for Theoretical and Computational Chemistry at the European Association of Chemical and Molecular Sciences (EuCheMS former FECS)
Yaroslav the Wise State University of Novgorod the Great
Division for Computational Chemistry at the D.I. Mendeleev Chemical Society of Russia
A.N. Frumkin Institute of Physical chemistry and Electrochemistry RAS
Independent University of Moscow

17-th V.A.Fock Meeting on Quantum, Theoretical and Computational Chemistry.
23-27.08.2021, Novgorod, Russia

BOOK OF ABSTRACTS
of the 17-th V.A. Fock Meeting on Theoretical, Quantum and Computational Chemistry

A.L. Tchougréeff — Editor

Novgorod the Great

2021

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Tentative Schedule

Monday August, 23st - Friday August, 27th

Time	Mon	Tue	Wed	Thu	Fri
9.00-10.00	Arrivals	Kvashnin L 2263	Zakharov L 2277	Medvedev L 2298	Tchougreeff L 2286
10.00-10.30		Yuldasheva O 2284	Gerasimov O 2292	Broer L 2307	Chaliy O 2295
10.30-11.00		Coffee break	Coffee break	Coffee break	Coffee break
11.00-12.00		Onishi L 2304	Evarestov L 2282	Maltsev L 2300	Bezrukov L 2268
12.00-12.30	Registration	Kozlov O 2287	Kiselev O 2293	Tupitsyn L 2301	Kvashnin O 2302
12.30-14.00	Opening 13:45	Lunch	Lunch	Lunch	Lunch
14.00-15.00	Ignatov L 2262	Rassolov L 2272	Boat Trip	Larin O 2305	General discussion and Closing
15.00-15.30	Demidov O 2289	Grushevskaya O 2276		Poster presentations	
15.30-16.00	Coffee break	Coffee break		Coffee break	Departures
16.00-16.30	Gorn O 2278	Malyshev O 2290		Posters	
16.30-17.00	Sudarkova O 2280	Popov O 2291			
17.00-17.30	Losev O 2296	Vyboishchikov O 2270			
18.00-20.00	Welcome Party		Conference Dinner		

Development of approaches for modeling ESR spectra of matrix-isolated atoms

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ESR spectroscopy is one of the most widely used approaches to studying matrix-isolated atoms with unpaired electrons. Experimental data for a large number of systems are described in the literature. The most studied to date is the H @ RG system. Based on these data, it was established that the matrix environment affects both the position of the lines in ESR spectra, which is determined primarily by the hyperfine interaction constant and the linewidth.

The problem of the theoretical description of these parameters of the ESR spectrum for a system of a matrix-isolated hydrogen atom has been the subject of a large number of theoretical works, from the first semi-empirical estimates of Adrian to the study of Dmitriev in 2020. While good agreement between theoretical and experimental predictions has been achieved for the Ar, Kr, Xe system, the question with neon is still open. In more complex systems, the results are even more nontrivial.

In this work I would like to present the progress made by our research group towards modeling the ESR spectra of matrix-isolated systems. Based on the proposed and developed approach to obtaining thermodynamically stable structures of matrix-isolated atoms, we were able to obtain parameters describing the geometric structure of matrix-isolated atoms. Based on a combination of DIM approaches and molecular dynamics methods, we proposed a method for calculating the position and widths of the ESR spectra bands. To validate the additive approximation of the electron density shift near the nucleus, which is responsible for the Fermi-contact interaction, we performed precision calculations of these parameters using the linear response theory. The approaches obtained were applied to describe the matrix-isolated H, Li, and Na atoms. The results obtained were discussed in comparison with the known experimental data and made it possible to determine the undescribed trapping sites.

The author is grateful to the Russian Science Foundation for the financial support under Project 17–13–01466.