



Шаповалова Светлана Олеговна
Международная исследовательская
лаборатория функциональных
наноматериалов

Должность: Научный сотрудник
Email: scherkasova@sfnedu.ru

Дата рождения: 08.07.1994 г.,
с. Кинель-Черкассы, Россия

Должности:

2014-2018 гг.: ЮФУ, физический факультет, кафедра физики наносистем и спектроскопии, старший лаборант.

2018-2023 гг.: ЮФУ, Институт интеллектуальных материалов, инженер.

2023 – н.в.: ЮФУ, Институт интеллектуальных материалов, научный сотрудник.

Образование и ученые степени:

2016 г.: бакалавриат 03.03.02 Физика, физический факультет, Южный федеральный университет, Ростов-на-Дону, Россия;

2018 г.: магистратура 03.04.02 Физика, Институт интеллектуальных материалов, Южный федеральный университет, Ростов-на-Дону, Россия;

2022 г. : к.ф.-м.н. Институт интеллектуальных материалов, Южный федеральный университет, Ростов-на-Дону, Россия. Тема диссертации: "Диагностика локального атомного окружения, спинового и зарядового состояния ионов переходных металлов для создания фотоактивных материалов".

Направления исследований (ключевые слова):

Спин-кроссоверы, переходные металлы, XANES, квантово-химические расчеты.

Участие в конференциях:

- XAFS 2021 – 18th International Conference on X-Ray Absorption Fine Structure 2021, 11 - 13 Июль 2021, устный доклад - Temperature and time-resolved XANES studies of novel valence tautomeric cobalt complex; постерный доклад - XAS

diagnostic of the photoactive state in Co(II) azobenzene complex in organic solutions.

- IUCr 2021 - 25th Congress of the International Union of Crystallography, 14-22 Август 2021, постерный доклад - Temperature and time-resolved XANES studies of novel valence tautomeric cobalt complex.
- IWSN2021 – International Workshop on Synchrotron and Neutron Radiation 6-7 декабря, 2021, Ростов-на-Дону, устный доклад - Characterization of novel valence tautomeric cobalt complex using temperature- and time-resolved XANES studies.

Участие в экспериментах на синхротронах:

2021 г.: Курчатовский институт синхротронных исследований (Москва, Россия) – Магнитная бистабильность 3,6-ди-трет-бутил-катехолатных комплексов железа(III) с трис-(2-пиридилметил)амином.

2018 г.: Европейский синхротронный центр ESRF (Гренобль, Франция) – Operando XAS/XRD study of mixed d-metal olivines as a new cathode material for modern Li-ion batteries.

2017 г.: Европейский синхротронный центр ESRF (Гренобль, Франция) – Comparative study of CO oxidation on Au-Cu nanoparticles formed in crystalline and amorphous porous silicalites.

Область научных интересов:

Исследования в области спин-кроссоверов и комплексов с валентной таутомерией; проведение низкотемпературных экспериментов методами XANES и оптической спектроскопии. исследованию структуры и свойств переходных металлов, являющихся частью систем (композит/комплекс) для создания каталитическиактивных материалов; установление взаимосвязи между параметрами локальной атомной и электронной структуры ионов переходных металлов, их спинового состояния и оптическими свойствами композитных материалов и молекулярных комплексов на их основе.

Методы:

Спектроскопия рентгеновского поглощения, DFT расчеты, термогравиметрический анализ, оптическая спектроскопия, масс-спектрометрия с индуктивно-связанной плазмой

Российские гранты:

2020-2022 гг.: РФФИ «Аспиранты» «Изучение новых комплексов 3d металлов с валентной таутомерией при влиянии температуры и излучения» .

Научные публикации в реферируемых журналах:

1. Influence of Strong pi-Acceptor Ligands on Cr-K-edge X-Ray Absorption Spectral Signatures and Consequences on Interpretation of Surface Sites in the Phillips Catalyst. Yuya Kakiuchi, Svetlana Shapovalova, Bogdan Protsenko, Sergey Guda, Olga V. Safonova, Alexander Guda, Christophe Copéret, Inorganic Chemistry, 2023, 10, DOI: 10.26434/chemrxiv-2023-9ggbk

2. 1,10-Phenanthroline-5,6-dione-bridged FeCo complexes: a DFT investigation of the electronic lability. Starikov, A.G., Starikova, A.A., Shapovalova, S.O., Guda, A.A., Soldatov, A.V. *Structural Chemistry*, 2023, 34(4), pp. 1279–1288
3. Influence of mechanical activation on crystal structure and physical properties of YbFeO₃ Li, Z., Abdulvakhidov, K., Abdulvakhidov, B., A. Soldatov, A. Nazarenko, P. Plyaka, A. Manukyan, V. J. Angadi, S. Shapovalova, M. Sirota, M. Vitchenko, I. Mardasova, E. Ubushaeva, Kallaev, S., Omarov, Z. *Applied Physics A: Materials Science and Processing*, 2022, 128(12), 1075
4. Spin transitions in ferric catecholate complexes mediated by outer-sphere counteranions. Chegerev, M., Demidov, O., Vasilyev, P., N. Efimov, S. Kubrin, A. Starikov, V. Vlasenko, A. Piskunov, S. Shapovalova, A. Guda, Rusalev, Y., Soldatov, A. *Dalton Transactions*, 2022, 51(29), pp. 10909–10919
5. Temperature and Time-resolved XANES Studies of Novel Valence Tautomeric Cobalt Complex. Shapovalova, S.O., Guda, A.A., Bubnov, M.P., G. Smolentsev, Yu.V. Rusalev, V.V. Shapovalov, A.A. Zolotukhin, V.K. Cherkasov, A.G. Starikov, Vlasenko, V.G., Soldatov, A.V. *Chemistry Letters*, 2021, 50(11), pp. 1933–1937
6. Photoswitchable zirconium mof for light-driven hydrogen storage. Butova, V.V., Burachevskaya, O.A., Podshibyakin, V.A., E.N Shepelenko, A.A. Tereshchenko, S.O. Shapovalova, O.I. Il'in, Bren', V.A., Soldatov, A.V. *Polymers*, 2021, 13(22), 4052
7. XAS Diagnostic of the Photoactive State in Co(II) Azobenzene Complex in Organic Solvents. Vlasenko, V.G., Shapovalova, S.O., Guda, A.A., A.V. Chernyshev, A.G. Starikov, G.Yu. Smolentsev, A.S. Burlov, Mashchenko, S.A., Soldatov, A.V. *ChemistrySelect*, 2021, 6(28), pp. 7087–7092
8. The Influence of Acetic Acid on the Properties of Microporous Metal–organic Framework MIL-88a at Microfluidic Conditions and room Temperature. Medvedev, P.V., Butova, V.V., Soldatov, M.A., A. A. Kuzharov, A. G. Fedorenko, S. O. Shapovalova (Cherkasova), O. A. Burachevskaya, Gorban, I.E., Soldatov, A.V. *Nanobiotechnology Reports*, 2021, 16(4), pp. 488–496
9. Theoretical and experimental characterization of Cu-doped amorphous silicate glass. Tsureyan, A.A., Cherkasova, S.O., Budnyk, A.P. *Journal of Molecular Structure*, 2020, 1205, 127629
10. One-pot sol-gel synthesis of porous silica glass with gold nanoparticles. Budnyk, A.P., Cherkasova, S.O., Damin, A. *Mendeleev Communications*, 2017, 27(5), pp. 531–534



Shapovalova Svetlana Olegovna

Born: 08.07.1994, Russia

Address: Southern Federal University, 178/24 Sladkova str., Rostov-na-Donu, 344090 Russia.

Email : scherkasova@sfedu.ru

Website: <http://nano.sfedu.ru>

Academic positions:

2014-2018 - SFedU, Physics Department, Department of Physics of Nanosystems and Spectroscopy, Senior Laboratory Assistant.

2018-2023 - SFedU, The Smart Materials Research Institute, Engineer.

2023 – present - SFedU, The Smart Materials Research Institute, Scientist.

Education and Degrees:

Bachelor degree (2016): 03.03.02 Physics, Physics Department, Southern Federal University, Rostov-on-Don, Russia;

Master degree (2018): 03.04.02 Physics, The Smart Materials Research Institute, Southern Federal University, Rostov-on-Don, Russia;

PhD in Physics (2022): The Smart Materials Research Institute, Southern Federal University, Rostov-on-Don, Russia. PhD thesis title "Diagnostics of the local atomic environment, spin and charge states of transition metal ions for the creation of photoactive materials".

Research sectors (Keywords) - spin crossovers, transition metals, XANES, quantum chemical calculations.

Participation in conferences:

1. XAFS 2021 – 18th International Conference on X-Ray Absorption Fine Structure 2021, 11 - 13 July 2021, oral presentation - Temperature and time-resolved XANES studies of novel valence tautomeric cobalt complex; poster presentation - XAS diagnostic of the photoactive state in Co(II) azobenzene complex in organic solutions.
2. IUCr 2021 – 25th Congress of the International Union of Crystallography, 14-22 August 2021, poster presentation - Temperature and time-resolved XANES studies of novel valence tautomeric cobalt complex.

3. IWSN2021 – International Workshop on Synchrotron and Neutron Radiation 6-7 December 2021, Rostov-on-Don, oral presentation - Characterization of novel valence tautomeric cobalt complex using temperature- and time-resolved XANES studies.

Participation in experiments at synchrotrons:

2021 – Kurchatov Institute for Synchrotron Research (Moscow, Russia) – Magnetic bistability of 3,6-di-tert-butyl-catecholate complexes of iron(III) with tris-(2-pyridylmethyl)amine.

2018 – European Synchrotron Radiation Facility ESRF (Grenoble, France) – Operando XAS/XRD study of mixed d-metal olivines as a new cathode material for modern Li-ion batteries.

2017 – European Synchrotron Radiation Facility ESRF (Grenoble, France) – Comparative study of CO oxydation on Au-Cu nanoparticles formed in crystalline and amorphous porous silicalites.

Fields of interest:

Research interests include research in the field of spin crossovers and complexes with valence tautomerism; conducting low-temperature experiments using XANES and optical spectroscopy methods. study of the structure and properties of transition metals that are part of systems (composite/complex) for the creation of catalytically active materials; establishing the relationship between the parameters of the local atomic and electronic structure of transition metal ions, their spin state and the optical properties of composite materials and molecular complexes based on them.

Methods:

X-ray absorption spectroscopy, DFT calculations, thermogravimetric analysis, optical spectroscopy, inductively coupled plasma mass spectrometry.

Scientific publications in referred journals:

1. Influence of Strong pi-Acceptor Ligands on Cr-K-edge X-Ray Absorption Spectral Signatures and Consequences on Interpretation of Surface Sites in the Phillips Catalyst. Yuya Kakiuchi, Svetlana Shapovalova, Bogdan Protsenko, Sergey Guda, Olga V. Safonova, Alexander Guda, Christophe Copéret, *Inorganic Chemistry*, 2023, 10, DOI: 10.26434/chemrxiv-2023-9ggbk.
2. 1,10-Phenanthroline-5,6-dione-bridged FeCo complexes: a DFT investigation of the electronic lability. Starikov, A.G., Starikova, A.A., Shapovalova, S.O., Guda, A.A., Soldatov, A.V. *Structural Chemistry*, 2023, 34(4), pp. 1279–1288.
3. Influence of mechanical activation on crystal structure and physical properties of YbFeO₃ Li, Z., Abdulvakhidov, K., Abdulvakhidov, B., A. Soldatov, A. Nazarenko, P. Plyaka, A. Manukyan, V. J. Angadi, S. Shapovalova, M. Sirota, M. Vitchenko, I. Mardasova, E. Ubushaeva, Kallaev, S., Omarov, Z. *Applied Physics A: Materials Science and Processing*, 2022, 128(12), 1075.
4. Spin transitions in ferric catecholate complexes mediated by outer-sphere counteranions. Chegrev, M., Demidov, O., Vasilyev, P., N. Efimov, S. Kubrin, A.

- Starikov, V. Vlasenko, A. Piskunov, S. Shapovalova, A. Guda, Rusalev, Y., Soldatov, A. Dalton Transactions, 2022, 51(29), pp. 10909–10919.
5. Temperature and Time-resolved XANES Studies of Novel Valence Tautomeric Cobalt Complex. Shapovalova, S.O., Guda, A.A., Bubnov, M.P., G. Smolentsev, Yu.V. Rusalev, V.V. Shapovalov, A.A. Zolotukhin, V.K. Cherkasov, A.G. Starikov, Vlasenko, V.G., Soldatov, A.V. Chemistry Letters, 2021, 50(11), pp. 1933–1937.
 6. Photoswitchable zirconium mof for light-driven hydrogen storage. Butova, V.V., Burachevskaya, O.A., Podshibyakin, V.A., E.N Shepelenko, A.A. Tereshchenko, S.O. Shapovalova, O.I. Il'in, Bren', V.A., Soldatov, A.V. Polymers, 2021, 13(22), 4052.
 7. XAS Diagnostic of the Photoactive State in Co(II) Azobenzene Complex in Organic Solvents. Vlasenko, V.G., Shapovalova, S.O., Guda, A.A., A.V. Chernyshev, A.G. Starikov, G.Yu. Smolentsev, A.S. Burlov, Mashchenko, S.A., Soldatov, A.V. ChemistrySelect, 2021, 6(28), pp. 7087–7092.
 8. The Influence of Acetic Acid on the Properties of Microporous Metal–organic Framework MIL-88a at Microfluidic Conditions and room Temperature. Medvedev, P.V., Butova, V.V., Soldatov, M.A., A. A. Kuzharov, A. G. Fedorenko, S. O. Shapovalova (Cherkasova), O. A. Burachevskaya, Gorban, I.E., Soldatov, A.V. Nanobiotechnology Reports, 2021, 16(4), pp. 488–496.
 9. Theoretical and experimental characterization of Cu-doped amorphous silicate glass. Tsaturyan, A.A., Cherkasova, S.O., Budnyk, A.P. Journal of Molecular Structure, 2020, 1205, 127629.
 10. One-pot sol-gel synthesis of porous silica glass with gold nanoparticles. Budnyk, A.P., Cherkasova, S.O., Damin, A. Mendeleev Communications, 2017, 27(5), pp. 531–534.

Russian national grants:

2020-2022 RFBR "Graduate Students" "Study of new complexes of 3d metals with valence tautomerism under the influence of temperature and radiation".