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| University | Samara National Research University |
| Level of English | Fluent |
| Field of study and degree program of the doctoral student to be admitted | 1.4.1 Inorganic Chemistry |
| Research projects of the potential research supervisor | |
| Suggested topics for research | <ul style="list-style-type: none"> • Synthesis, study of the structure and properties of new coordination compounds. • Analysis of the coordination features of various ligands. • Application of Voronoi–Dirichlet polyhedra to study the structure of crystals. • Search for relationships between composition, structure and properties within the framework of the stereoatomic model of crystal structures. |
|  <p>Research supervisor: Denis V. Pushkin, Doctor of Science at Samara State University</p> | <i>Inorganic and nuclear chemistry</i> |
| | <p>Supervisor's research interests: Synthesis and study of the structure and properties of new coordination compounds. Study of the relationship between the composition/structure/properties of solids. Use and development of the stereoatomic model of crystal structures and Voronoi–Dirichlet polyhedra for the analysis of the structure of crystals. Study of noncovalent interactions, the phenomenon of polymorphism, actinide contraction, the electron-donating ability of ligands, the stereo effect of a lone electron pair, etc. Study of the fundamental principles of the formation of solids and universal approaches to the description of chemical bonds, determination of the oxidation states of elements, coordination numbers of atoms, geometric characteristics of molecules, etc.</p> |
| | <p>Distinctive characteristics of research (if any)</p> <ul style="list-style-type: none"> • Professional, responsive and collaborative research team. • The unique advanced software for the analysis of crystalline substances, which has no analogues in the world, is used. • The research team constantly participates in the implementation of work on grants that receive financial support. • Interaction with leading Russian and foreign scientists working in the field of interests of the scientific group. • Experimental work is carried out on high-tech equipment from the centers of collective use. • The results of scientific work are constantly published in highly cited scientific journals and reported at leading specialized international conferences. |

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| | <p>Requirements of the potential research supervisor (if any) None</p> <p>Key publications of the potential research supervisor <i>Total amount of scientific articles published in journals, indexed in Web of Science, Scopus, RSCI, for the last 5 years: 12.</i> Karasev M.O., Karaseva I.N., Pushkin D.V., Kurbatova S.V. Non-Covalent Interactions in α- and β-Imidazole Structures // Journal of Structural Chemistry 2025. — Vol. 66. Issue 1. № 1. — P. 97-107. Mitina D.S. Serezhkina L.B., Grigoriev M.S., Pushkin D.V., Serezhkin V.N. Imidazolium and 2-Methylimidazolium Iodoacetatouranylates: Structure and Some Properties // Russian Journal of Physical Chemistry A 2024. — Vol. 98. Issue 1. № 1. — P. 113-119. Mitina D.S. Serezhkina L.B., Grigoriev M.S., Pushkin D.V., Serezhkin V.N. Lithium, Sodium, and Strontium Fluoroglutaratouranylates: Structure and Some Properties // Radiochemistry 2024. — Vol. 66. Issue 2. № 2. — P. 125-133. Karasev M.O., Fomina V.A., Karaseva I.N., Pushkin D.V. Crystallochemical Role of Benzoate and Phenylacetate Ions in Structures of Coordination 3d-Metal Compounds // Russian Journal of Coordination Chemistry. 2023. — Vol. 49. Issue 4. № 4. — P. 247-256 Uhanov A.S., Sokolova M.N., Fedoseev A.M., Bessonov A.A., Nechaeva O.N., Savchenkov A.V., Pushkin D.V. New Complexes of Actinides with Monobromoacetate Ions: Synthesis and Structures. (2021) ACS Omega, 6, pp. 21485–21490.</p> |
| | <p>Intellectual property outputs (if any) Results of intellectual activity For the first time, more than fifty new uranyl carboxylates were obtained, the structure of their crystals was determined and it was proved that more than twenty of them possess nonlinear optical activity. The use Voronoi-Dirichlet polyhedra for the first time allowed to explain some features of thermal polymorphism of actinides, as well as to justify the crystal-chemical criteria for the presence of 5f-binding interactions between actinide atoms. The presence of a quantitative relationship between the nonlinear optical activity of U(VI) triscarboxylates and the value of a vector characterizing the displacement of the nucleus of a uranium atom from the center of gravity of its Voronoi-Dirichlet polyhedron in a cationic sublattice of uranium atoms and external sphere single or doubly charged cations was shown. The principle of maximum space filling was validated in sublattices containing actinide atoms (from Th to Es) in the structures of all studied to date crystalline substances. It was found that in U-sublattices of substances having 20 or more crystallographically nonequivalent U atoms in the unit cell, the short-range (or crystal-chemical) order in the mutual arrangement of atoms is</p> |

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| | <p>absent and only the long-range order is preserved (translational symmetry). The analysis of coordination polyhedra MC_n (M - s-metal, B or Al) in the structures of organoelement compounds was conducted. It was established that the volume of Voronoi-Dirichlet polyhedra of M atoms is almost independent of their coordination numbers.</p> <p>Patent # RU 2 570 236 C1 Date of publication: 10.12.2015 Bull. № 34 Method of obtaining calibration mixtures by photochemical reaction of potassium carboxylatouranylates and device for its realisation Savchenkov A.V., Pushkin D.V., Serezhkina L.B., Arutjunov J.I., Serezhkin V.N.</p> |
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