Annotation of scientific works nominated for the St. Petersburg State University award in 2021

Title:

Computer modeling and theoretical studies in organic, inorganic, and organometallic chemistry: non-covalent interactions, reactivity and catalysis

Name, academic degree and position of the author:

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Computer modeling can help experimental chemists in studying of the structure, properties, and reactivity of a wide range of organic, inorganic, and organometallic compounds. To date, in quantum chemistry, computer modeling has almost completely replaced the traditional analytical mathematical methods of calculation. Computer modeling allows in some cases to predict previously unobservable chemical phenomena, it actually represents a new way of conducting research in chemistry – a computer experiment.

Scientific works in the field of computer modeling, nominated for this award, are devoted to the application of modern advanced quantum chemical and computational methods (*ab initio* and DFT) as well as some special techniques (e.g., topological analysis of electron density distribution, natural bond orbital analysis, charge decomposition analysis, basis sets superposition error correction, isodesmic reactions, HSAB principle theoretical model, Hirshfeld surface analysis) in the studies of following main lines: properties of organometallic and coordination compounds, their reactivity, and catalysis.

The major points are:

- Studying the nature of different non-covalent interactions (hydrogen, halogen and chalcogen bonding, stacking, metallophilic interactions et al.) and quantitative assessment of their energies – a paradigm of supramolecular chemistry and crystal engineering.

- Investigation of nucleophilic addition and cycloaddition reactions (their mechanisms,

driving forces, kinetics and thermodynamics), and other fundamental studies in theoretical chemistry (conformational transitions and barriers to the rotation of functional groups, the nature of chemical bonds, orbital and charge factors, photophysical properties of various compounds).

- Consideration of hydrocarbon oxidation processes promising for the oil and gas industry and their conversion to alcohols and epoxides.

The obtained results will be potentially useful for biochemistry (understanding the nature of proteins folding), medicine (synthesis of antibacterial, antiviral, and antitumor drugs and marks for neutron-capture therapy of oncological diseases), chemical industry and technology (catalysis of cross-coupling and multicomponent reactions and hydrocarbon conversion processes), materials science (design of smart materials with valuable redox, electronic, mechanical, magnetic and optical properties, promising for the manufacture of LEDs, photovoltaic cells of solar power plants, porous structures, sensors, battery cells, and liquid crystals).

These scientific works are interdisciplinary in nature and performed at the junction of theoretical and experimental chemistry, crystallography and materials science.