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## **Computational Insights into the Reactivity of S-Nitrosothiols**

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S-nitrosothiols (RSNOs), compounds containing an SNO functional group, play an important role in storage and transport of nitric oxide *in vivo*. The S–N bond in RSNOs possesses a number of very interesting properties: although weak (~30 kcal/mol) and elongated (~1.8 Å), it is also conformationally restricted, which suggests partial double-bond character. Moreover, its stability can be significantly altered by interaction with metal ions depending on the mode of coordination. Quantum-chemistry calculations published so far fail to provide a consistent description of RSNOs since the results greatly depend on the method used. In this talk, we will show how a combination of high-level *ab initio* calculations and Density-Functional Theory calculations, together with Natural Bond Orbital analysis and Natural Resonance Theory, reveal the reasons behind the unusual properties of RSNOs. We propose a concise and chemically intuitive resonance description of the RSNO electronic structure that rationalizes the reactivity of RSNOs and predicts their properties. The same resonance description also helps explain why many quantum chemistry methods fail to properly describe RSNOs.

Qadir Timerghazin received his undergraduate degree in Chemistry from Bashkir State University, Ufa, Bashkortostan, Russia, in 1997. He then pursued graduate studies in Physical Organic Chemistry at the Institute of Organic Chemistry, Ufa Research Centre of the Russian Academy of Science, where he received a PhD in 2000 for studies of reactions of ozone and chlorine dioxide with organic compounds. He then moved to Montréal, where he spent a few months at McGill University, studying atmospherically important reactions of chlorine and bromine atoms with Prof. Parisa A. Ariya, and earned a PhD in computational chemistry at Concordia University under the direction of Prof. Gilles H. Peslherbe, studying the structure, photochemistry and charge-transfer-to-solvent dynamics of anionic clusters. He spent one year as a postdoctoral fellow in the group of Prof. Ann M. English at Concordia University, where he studied the reactivity of S-nitrosothiols and modeled mass-spectrometry aspects of nitroxyl radicals, before moving to the University of Alberta in 2007 as an Alberta Ingenuity Postdoctoral Fellow, to study the photochemistry of fluorescent proteins under the direction of Prof. Alex Brown.

