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Postdoctoral Research Scientist Position

opened in the Department of Theoretical Chemistry at J. Heyrovský Institute of Physical Chemistry in Prague, Czech Academy of Sciences.

Summary
With support from the Czech Grant Agency (15-10279Y), **Dr. Martin Srnec offers one postdoctoral fellowship for 2016-2017**. The project, based on the use of large-scale multireference ab initio, DFT and other theoretical methods, aims at calculations of redox properties of nonheme iron active sites and elucidation of their effects on reactivities and selectivities with respect to a possible design of new catalysts.

Topic
Iron as the most abundant redox-active metal in biology catalyzes many vital processes by performing difficult chemical reactions such as functionalization of aliphatic C-H bonds. In this proposal, we will focus on mononuclear and binuclear nonheme iron (NHFe) enzymes and their model complexes. These species are important not only due to their functions in nature but also represent challenging systems for both experimental and theoretical chemistry. From the theoretical point of view, the requirement for an accurate description of their complex electronic structures often complicates predictions of their redox potentials and related reactivities. Nowadays, a theoretical protocol that would be of great interest for the appealing possibility to reliably predict redox potentials and reactivities of important but experimentally elusive NHFe species is not yet available. Besides developing such a protocol, the results are expected to contribute to understanding of the general factors that control selective mechanisms in the realm of powerful NHFe enzymes and related bio-inspired complexes.

More specifically, we offer to work on one of the following topics:

i) Theoretical protocol for calculations of redox potentials of bioinorganic complexes.
ii) Redox properties and reactivity of non-heme iron active sites.
iii) S-adenosylmethionine-dependent enzymes and mobility of radicals in enzymes

Eligibility
The candidate should be highly motivated, self-driven and passionate about science and hold a PhD degree (preferably) in theoretical (physical) chemistry (or chemical physics). An experience with application of quantum-chemical methods (including multireference ab initio and QM/MM methods) to bioinorganic and metalloenzymatic complexes, their spectroscopic and catalytic properties is desirable. Good communication and collaborative spirit and fluency in spoken and written English is required.

Employment Conditions
The competitive salary is offered and will be based on the candidate`s qualifications and experience. Contract type: 12 months, with possibility for extension depending on performance. Expected start date is preferably in February/March 2016 or upon agreement. The position is not associated with any teaching obligations.

Application Materials
Please send application (including CV, publications, short statement of research background/interests and if possible the contact information of a reference/references) by email to Dr. Martin Srnec at **srnec@jh-inst.cas.cz**. To obtain further information about the position please contact Dr. Martin Srnec.

Representative Publications Related to the Topic.

1/ Srnec, M.; Chalupský. J.; Kývala, M.; Rulíšek L. et al. *J. Am. Chem. Soc.*, 2008, *130*, 10947-10954.

2/ Srnec, M; Wong, S. D.; England, J.; Que Jr.; L.; Solomon, E. I. *Proc. Nat. Acad. Sci. USA*, 2012, *109*, 14326-14331.

3/ Wong, S. D., Srnec, M.; Solomon, E. I et al. *Nature* 2013, 499, 320-323.

4/ Chalupský, J.; Rokob, T. A.; Rulíšek, L.; Srnec, M. et al. *J. Am. Chem. Soc.* 2014, *136*, 15977-15991.

5/ Bím, D.; Rulíšek, L.; Srnec, M. *J. Phys. Chem. Lett.* 2016, *7*, 7-13.

13. 1. 2016 RNDr. Martin Srnec, PhD.

Theoretical Bioinorganic Chemistry: