

28 Aug 2018

**Evaluation of habilitation thesis of Dr. Lubomír Rulíšek:
“Modeling Physico-Chemical Properties of Bioinorganic Systems”**

The candidate presents in the thesis 20 publications and an introductory summary that puts the papers into a wider context and provides a brief discussion on the challenges associated with this kind of modeling. The work covers three main themes: 1) Modeling of metalloenzymes, 2) Modeling of metal-ion selectivity in peptides, and 3) Computation of electrochemical properties of bioinorganic systems.

The field of theoretical bioinorganic chemistry is a truly multidisciplinary one that requires deep knowledge not only the various quantum chemical techniques and electronic structure methods, but also in many experimental fields such as organic, inorganic, physical, and biological chemistry, as well as a number of different spectroscopic methods. The thesis demonstrates that Dr. Rulíšek has acquired a unique expertise that allows him to tackle important and difficult problems in the field.

The work is of consistently high quality, characterized by insightful choice of projects with the aim of gaining deep understanding. Both the summary and the included papers are clearly written and easy to follow, despite the fact that the problems addressed are very complex.

One particularly attractive aspect of the thesis is the close collaborative nature of the work with leading experimental partners. Paper V on the identification of the peroxy adduct in multi-copper oxidases, Paper VII on the design of metal-binding peptides, and Paper XI on the spectroscopic properties of Δ^9 desaturase are excellent examples of these fruitful collaborations.

In conclusion, there is no doubt in my opinion that Dr. Rulíšek has made significant contributions to the field of theoretical bioinorganic chemistry. He is a very active member of the community and the presented work is at the international research forefront. I can therefore strongly recommend him for the promotion to Associate Professor.

Sincerely Yours
Fahmi Himo

Professor of Quantum Chemistry