Tentative Outline

Special Issue for Current Organic Chemistry

Guest Editor(s): Martin Korth

TITLE: Recent methodological developments in the atomic-scale modelling of bioorganic interactions

Aims & Scope:

Modelling bioorganic interactions is of high importance for understanding processes in biochemistry and life science as a whole. The last decade has seen tremendous efforts at reaching to higher accuracy and wider applicability of modelling techniques. As a result, complicated problems like photodynamics, quantum-level structure refinement, and highly-accurate energetics of biologically relevant systems have now come into the reach of computational approaches. It can be expected that such theoretical approaches, in close cooperation with experiment, will become more and more important for gaining insight into complex biological processes. The proposed minithematic issue aims at giving an overview of how advanced techniques allow to make progress on such 'hard' problems. As contributors I would like to invite five young researchers who have made important contributions and who are expected to contribute substantially to further progress in the field also in the future. The contributors will be asked to summarize their field in a way that a general chemistry audience will understand the central problems and the basic ideas of how they are approached by leading researchers in the field. Emphasis should be given to an easy-to-understand introduction into the basics, while the full complexity should be illuminated only at the end of the review as an outlook. Advanced readers should find the articles useful as a good starting point for getting a complete overview of the respective field. Further contributors could be invited, contributions from five authors are already secured, see list of possible contributors below for titles and complete affiliations.

Subtopics:

- Electronic excitations in protein environments
- X-ray crystal structure determination with quantum-chemical methods
- Excited states relaxation in biological systems
- Highly-accurate energetics of (bio)organic interactions
- Photodynamics with QM/MM methods

Approximate Schedule:

- Acceptance of proposal: August 2015
- Manuscript Submission Deadline: + 4 months from acceptance
- Peer Review Due: + 1 month
- Revision Due: + 2 weeks
- Notification of Acceptance by the Guest Editor: + 1 week
- Final Manuscript Due: + 1 week
- Complete issue submitted: February 2016