Kemijski inštitut
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VABILO NA PREDAVANJE / INVITATION TO THE LECTURE

Dr. Ernst-Walter Knapp

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Institute of Chemistry & Biochemistry
Macromolecular Modeling and Simulation of Biomolecular Systems
Fabeckstrasse 36A, Berlin, Germany (email: knapp@chemie.fu-berlin.de)

Sreda / Wednesday, 18. 9. 2013 ob / at 13:00

Velika predavalnica Kemijskega inštituta /
Lecture Hall at the National Institute of Chemistry
Hajdrihova 19, Ljubljana

Marriage of quantum chemistry and electrostatic to compute accurate pKa's and redox potentials in solution and proteins

Electron and proton transfer (ET, PT) processes are the most elementary chemical reactions in proteins. PT processes occur between titratable groups (Glu, Asp, His, Arg, Lys). ET processes involve redox-active compounds, which can be organic molecules or often transition metal complexes (TMC) appearing as cofactors in proteins. To characterize these processes energetically we need to know pKA values and redox potentials of these compounds with an accuracy of one pH unit or 50 mV, respectively. If experimental values are available for model compounds in solution we can compute the shift between solvent and protein environment just by evaluating electrostatic energies. But, in some particular important cases such model compounds are not available or their redox potentials or pKA are not known. Hence, accurate and generally applicable methods for ab initio computations of redox potentials and pKA values are needed. Until recently ab initio methods were not accurate and general enough to match these requirements. We have developed a combination of quantum chemical and electrostatic energy computations, which tries to solve this problem. For pKA values high level DFT methods combined with tuned electrostatic methods are appropriate. For the computation of redox potentials DFT alone is not appropriate. Therefore, we use for redox-active organic compounds an MP2 approach with post SCF correction term (G3MP2), while for transition metal complexes we use DFT with an adjusted functional and post SCF correction combined with electrostatic energy computation.

Vljudno vabljeni! / Kindly invited!

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