

- c hemisch
- p hysikalische
- g esellschaft

Gegründet im Jahre 1869 von H. Hlasiwetz,  
J. Loschmidt, J. Petzval und J. Stefan

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## EINLADUNG

zum Vortrag

von

**Prof. Pavel Hobza**

Institute of Organic Chemistry and Biochemistry  
Academy of Sciences of the Czech Republic

über

**Stability and function of biomacromolecules in  
relation to the interaction between their building  
blocks - a quantum chemical study**

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**Dienstag, 27. November 2007, um 17.30 Uhr**

Ort: Großer Hörsaal der Experimentalphysik, Universität Wien,  
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5, 1. Stock

**Abstract:**

Structures and stabilization energies of H-bonded and stacked structures of DNA base pairs and amino acid pairs are studied using the CCSD(T) and SAPT calculations. Resulting stabilization energies of H-bonded and stacked pairs are very large, much larger than considered before. This is especially true about stacked DNA base pairs and amino acid pairs. Stabilization energy of these structures originates exclusively in London dispersion energy and only high-level wave function theories can be applied. It is shown that stability of DNA double helix is mainly due to stacking interactions of nucleic acid bases while H-bonding is playing the role in molecular recognition.

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**CHEMISCH-PHYSIKALISCHE GESELLSCHAFT**

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Vorsitzender 2006/07: Ao.Univ.Prof. Dr. Wolfgang Linert, Institut für Angewandte Synthesechemie, Techn.Univ. Wien