chemisch
physikalische
gesellschaft

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

EINLADUNG

zum Vortrag

von

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über

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

am

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.