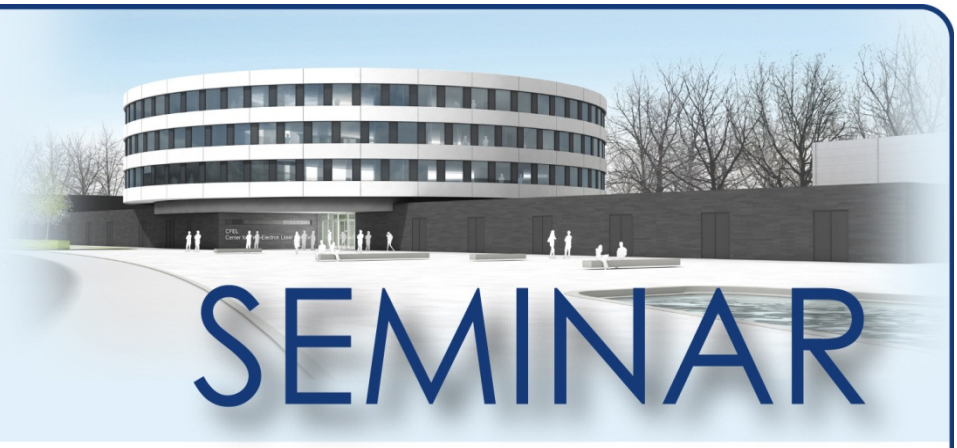
CFEL SCIENCE



SEMINAR

26th July 2017 - 13:30h

CFEL – Building 99, seminar room III (ground floor)

Andrei Duchko

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Numerical investigation of analytical properties of vibrational and rovibrational energy functions for different molecules

The main purpose of the research was to analyze analytical properties of energy, which is considered as a complex-valued function, depending on the perturbation parameter. These properties provide an effective way to improve perturbation theory methods for vibrational and rovibrational energy calculations. This analysis was made for different types of molecules and helped us to find and classify singularities of the energy function, determine the dependence of them on the convergence of corresponding perturbation series, i.e. signs and values of high order coefficients. Relations between resonances and singular points were studied and technique of calculation, neglecting the effect of resonances in energy spectrum was proposed. Different divergent series resummation techniques were tested and it was found that Pade-Hermite multivalued algebraic approximants show the best results due to their properties of reproducing several branches of multivalued function. Different techniques, such as repartioning were implemented to transform perturbation series and to improve their convergence. These analysis was implemented to design the technique, based on Rayleigh-Schrodinger perturbation theory and Pade-Hermite approximants, which helps to calculate vibrational and rovibrational energy levels for highly excited states. The proposed method was tested on different molecules both with model and high-precision potential surfaces.

Host: Jochen Küpper/ CFEL Molecular Physics Seminar