MO 31 Poster: Molecular Dynamics

Zeit: Dienstag 16:30–18:30 Raum: Labsaal

MO 31.1 Di 16:30 Labsaal

Numerical Examination of Beyond-Born-Oppenheimer Dynamics in the Hydrogen Molecular Ion — •Stefan Pieper and Manfred Lein — Max-Planck-Institute for Nuclear Physics, Heidelberg

An H_2^+ molecular ion (1+1 D) is exposed to a short intense laser pulse. The time dependent Schrödinger Equation is solved numerically on a 2D grid that is split into an inner and outer part. For large values of the electronic coordinate, the wave function is decomposed in products of electronic and nuclear wave functions, and the electron is assumed to move in a fixed effective potential, so that the two degrees of freedom can be treated independently. As a consequence, the numerical effort is significantly reduced and the electronic grid can be larger than 10^4 a.u. This enables one to keep the full wave function on the grid, even for pulses long enough to allow for substantial nuclear motion, and to examine kinetic-energy spectra of both the nuclei and the electron without loss of probability. In our approach we allow for wave packets being transferred in both directions between inner and outer region.

The 1D Coulomb interaction is modified beyond the usual soft core potential to account for the real motion of the electron in three dimensions, i.e. the Born-Oppenheimer potentials are reproduced more accurately for the two lowest lying states.

MO 31.2 Di 16:30 Labsaal

Nonlinear time series analysis of peptide dynamics — •Rainer Hegger, Alexandros Altis, and Gerhard Stock — J.W. Goethe Universität, Institut f. Physikalische und Theoretische Chemie, Marie-Curie Str. 11, 60439 Frankfurt

During the last few years the computer simulation of peptide dynamics has become feasible, by using an all-atom force field and an explicit or implicit representation of the solvent. Since the simulations produce a huge amount of data, it is of great importance to develop and improve suitable tools to analyze and interpret these data. As a new approach to this well-known problem, we suggest to apply the ideas originating from the theory of nonlinear dynamical systems to analyze molecular dynamics data. The goal is to develop mathematical models which, on one hand, are simple enough to be analyzed in great detail, and on the other hand, are realistic enough to reproduce the essential features of the dynamics.

In this work we present results obtained for small peptides (<=10 amino acids). By performing a PCA rotation in the space spanned by the dihedral angles of the peptide, we get rid of the dominant linear correlations between the peptide degrees of freedom. In the new coordinate system we are able to reveal the leading nonlinear properties.

By means of an analysis of these nonlinear properties we are able to describe the chaoticity of the system as a function of molecular properties, such as the length, the sequence and the types of residues of the peptide and thereby we obtain novel insight into the complexity and cooperativity of peptide folding.