



Electronic Structure of Rare Gas - Hydrogen Rydberg Molecules

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In recent decades excimers (molecules with repulsive ground states but chemically bound excited state) have become one of the major areas of research in laser physics and spectroscopy. In cases when the excited states are Rydberg states the excimers are also known as Rydberg molecules. Rydberg molecules are characterized by the Rydberg electron, which is far from the ion core, and a small ionisation potential. Due to the large radius of the Rydberg electron its interaction with the parent core should be regarded as approximately Coulombic.

Reliable potential energy curves and electron densities of the ground state and of the low lying excited states of rare gas - hydrogen Rydberg molecules have been calculated by using the configuration interaction method and large, flexible basis sets. The HeH and NeH Rydberg molecules have been studied as well in confinement. The influence of the applied potential on the structures and spectra of the ground and excited states of HeH and NeH has been investigated. The results of the studies will be presented and discussed.