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Long-range Molecules in Alkali Metals: Two-electron R-matrix method at intermediate nuclear distances

Ultra-long-range Rydberg molecules (ULRRMs) discussed in this talk consist of one atom in the highly excited Rydberg state and one or more distant atoms (~100 -- 10,000 a.u.) in their ground states. The bond between the Rydberg center and distant neutral atom is due to the scattering-like interaction between the Rydberg electron and neutral atom that modifies the phase of the Rydberg wave function so that the overall molecular electronic state is bound.

The mechanisms of the electronic bond in the diatomic ULRRMs will be introduced in this talk as well as the structure of their vibrational states. Their unusual properties (nodal character of the electronic wave function, oscillatory structures in the potential-energy curves, large dipole moment of the homonuclear diatomic molecules) will be discussed along with their use in the experiments.

Theoretical research of the ULRRMs at smaller internuclear separations (R~40 – 200 a.u.) will be introduced using an advanced model where the Rydberg electron interaction with the neutral perturber is parametrized in terms of the R-matrix that takes into account internal degrees of freedom of the perturber. The outlook for study of more complex perturbers using this approach will be mentioned.