The Role of Resonances in Molecular Rydberg States

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Molecular Rydberg states play an important role in a variety of collision processes. Recently the interest to molecular Rydberg states has increased due to theoretical prediction [1] that a certain class of molecular Rydberg states formed by interaction of a Rydberg atom with a ground-state Rb atom can be stable at very large internuclear separation, comparable to the size of the Rydberg atoms.

The properties of low-energy electron scattering by alkali-metal atoms are crucial for formation of such dimers. There are two distinct features: a virtual ^{3}S state and a ^{3}P shape resonance [2]. The ^{3}S and ^{3}P resonances lead to formation of local minima supporting localized vibrational states. The ^{3}S-dominated states were termed trilobite states [1] due to specific shapes of their wavefunctions.

In the present work [4], we use the Kirchhoff integral method [3] to calculate properties of the A*-B system, where A* is a Rydberg atom and B is a ground state alkali-metal atom. The e+A$^+$ interaction is included using Coulomb's Green function with the quantum defects. Interaction of the Rydberg electron with atom B is presented by a pseudopotential, which reproduces correct phase shifts from the Dirac R-matrix calculations and binding energies for corresponding negative ion. Analytical formulas for the wavefunction and dipole moment of trilobite state were derived. The obtained potential energy curves can be employed for calculation of inelastic processes in A-B collisions and for calculations of properties of long-range molecular Rydberg states. One of their most important features are dipole moments which appear due to orientation of Rydberg atom A in the presence of perturber B.

References

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