

Rydberg polyatomic molecules: Electronic structure and experimental proposal for their creation

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Synopsis We describe the electronic structure and main features of ultralong range Rydberg molecules formed by a Rydberg atom, either Rb or K, and the heteronuclear diatomic molecule KRb. By analyzing their electronic structure, we propose a protocol to create these molecules experimentally from a mixture of ultracold atoms and ultracold molecules.

The traditional Rydberg molecules are formed by a tightly bound positively charged core and an excited electron circulating around it. A more exotic type of Rydberg molecules were theoretically predicted to exist when a ground-state atom locally probes the Rydberg electronic wavefunction [1]. These ultralong-range exotic species were experimentally observed in 2010 [2], showing that, analogously to Rydberg atoms, they have a large sensitivity to external field, which allows their control. Another type of ultralong-range Rydberg molecules are theoretically predicted to exist if a heteronuclear diatomic molecule, a Λ -doublet or a rotating polar molecule, is immersed into the wave function of a Rydberg atom [3, 4, 5, 6]. The anisotropic scattering of the Rydberg electron from the permanent electric dipole moment of the polar molecule is responsible for the binding mechanism in these Rydberg molecules.

In this work, we describe the main properties of these exotic ultralong range Rydberg molecules formed by a Rydberg atom and a heteronuclear diatomic molecule. We explore the electronic structure of triatomic Rydberg molecules formed from a potassium or rubidium Rydberg atom and the KRb molecule. Our focus is on the interaction of Rydberg states, having s angular momentum, with ground and rota-

tionally excited KRb diatomic molecules. These Rydberg molecules could be created by exciting Rydberg atoms in a mixture of ultracold atoms and ultracold molecules, i.e., molecules such as K-KRb or Rb-KRb would be created experimentally. We have found adiabatic electronic states evolving from the Rydberg degenerate manifold with a significant contribution from a low angular momentum Rydberg state. These mixed electronic states are a few GHz deep and have several vibrational bound states [7]. We propose a protocol to create these molecules experimentally in these electronic states from a mixture of ultracold atoms and ultracold molecules [7].

References

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