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Ultralong-range Cs-RbCs Rydberg molecule: non-adiabaticity of dipole moments

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Triatomic ultra-long Rydberg molecules are formed by the interaction of a Rydberg atom, an excited atom with an electron with high principal quantum number, and a polar molecule. The study of Rydberg molecules is motivated by its interesting properties [1-3], and possible applications in ultracold chemical reactions [4] or quantum simulations [5]. In this work, we investigate the electronic structure and properties of the Rydberg molecule Cs-RbCs.

A complete study of the adiabatic electronic potentials has been performed. The rovibrational structure is described beyond the Born-Oppenheimer approximation, and the coupled Schrödinger equation is solved by including the non-adiabatic coupling terms of the neighbouring electronic potential curves. We explore the transition probabilities through the avoided crossing in the electronic structure, which characterize the ultracold chemical reaction of the Rydberg atom with the diatomic molecule. For the vibrational bound state, we provide the electric dipole moment and decay rates. For the experimental guidance, we identify the best states for photoassociation of this Rydberg molecules and provide the Franck-Condon factors.

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