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The building principle of triatomic trilobite Rydberg molecules[1]
PETER SCHMELCHER, CHRISTIAN FEY, FREDERIC HUMMEL, University of Hamburg — We explore the properties of triatomic ultralong-range Rydberg molecules consisting of two ground state atoms and a highly excited Rydberg atom. Our focus is on molecular states for which the Rydberg electron is in a superposition of high angular momentum states whose probability densities resemble the form of trilobite fossils. The associated potential energy landscape has an oscillatory shape and supports a rich variety of stable geometries with different bond angles and bond lengths. Based on an electronic structure investigation we analyze the molecular geometry systematically and develop a simple building principle that predicts the triatomic equilibrium configurations. As a representative example we focus on ^{87}Rb trimers correlated to the $n = 30$ Rydberg state. Using an exact diagonalization scheme we determine and characterize localized vibrational states in these potential minima with energy spacings on the order of 100 MHz.

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