Abstract Submitted
for the DAMOP14 Meeting of
The American Physical Society

Electronic structure of the paramagnetic and polar molecule RbSr[1] OLIVIER DULIEU, Laboratoire Aimé Cotton, CNRS/Univ. Paris-Sud/ENS Cachan, Orsay, France, PIOTR ŻUCHOWSKI, Instytut Fizyki, Uniwersytet Mikołaja Kopernika, Torun, Poland, ROMAIN GUÉROUT, Laboratoire Kastler-Brossel, CNRS, ENS, UPMC, Paris, France — We determine the electronic structure of RbSr, a molecule possessing both a permanent magnetic and electric dipole moment in its own frame allowing its manipulation with external fields at ultracold temperature. Two complementary ab-initio approaches are used: an approach relying based on optimized effective core potentials with core polarization potentials based on a full configuration interaction involving three valence electrons, and an approach using a small-size effective core potential with 19 explicitly correlated electrons in the framework of coupled-cluster theory. We have found excellent agreement between these two approaches for the ground state properties including the permanent dipole moment. We have focused on studies of excited states correlated to the two lowest asymptotes Rb(5p ^{2}P)+Sr(5s^2 ^{1}S) and Rb(5s ^{2}S)+Sr(5s5p ^{3}P) relevant for ongoing experiments on quantum degenerate gases. We present also the Hund c case potential curves obtained using atomic spin-orbit constants. These potential curves are an excellent starting point for spectroscopic studies of RbSr and of ultracold molecule formation processes.

[1]This work was supported in part by the National Science Foundation (Grant No. NSF PHY11-25915)

Olivier Dulieu
Laboratoire Aimé Cotton, CNRS/Univ. Paris-Sud/ENS Cachan, Orsay, France

Date submitted: 31 Jan 2014 Electronic form version 1.4