Internal cooling of cold Rb_2^+ ions with cold Rb atoms

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Synopsis The cooling of the internal degrees of freedom of cold Rb_2^+ ions induced by collisions with cold Rb atoms is modeled using a close-coupling approach. Due to the strong anisotropy of the potential energy surface, the process is predicted to be very efficient. Possible experimental implementation will be discussed.

The simultaneous trapping of cold atoms and cold ions in hybrid traps has opened new avenues for studying interactions in cold, dilute gas ensembles. In particular, molecular ion formation processes [1] have been investigated as a premise to ultracold chemistry. The molecular ions are generally obtained in a distribution of rotationally and vibrationally levels in their ground electronic state [2] which still remain to be cooled down to the lowest quantum level as required in many applications of single quantum state preparation.

Here we theoretically study the internal cooling of Rb_2^+ ions by ultracold Rb atoms, in the context of the recent experiment of Ref. [3].

A potential energy surface (PES) in standard atom-diatom Jacobi coordinates $V(R,r,\theta)$ has been calculated using a full configuration interaction approach, where the valence electrons of the individual atoms are represented by a relativistic effective core potential (ECP), corrected with core polarization potential (CPP) depending on the electronic angular momentum [4]. Thus, the Rb_3^+ system reduces to a two-electron problem, where the Hartree-Fock and the excitation determinants are computed in an atom-centered Gaussian basis set.

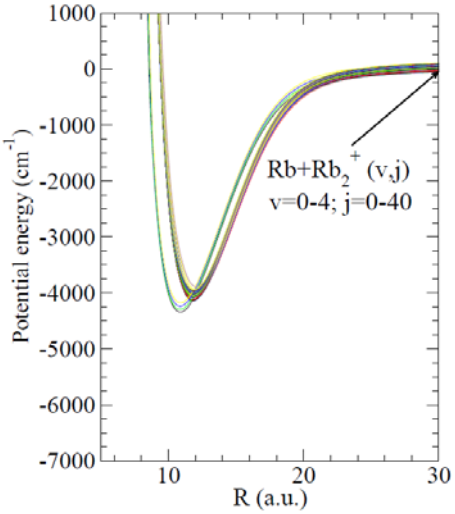

Figure 1. Rb-Rb_2^+ diabatic potential curves.

This PES is used to determine the interaction matrix in the asymptotic free rotor basis set $d^j_{m,0}(\theta)\chi_v(r)$ (rotational Wigner function $d^j_{m,0}(\theta)$ and vibrational wavefunction $\chi_v(r)$ of the diatom). The diagonal elements of the interaction matrix $V_{vj,v'j'}(R)$ (diabatic potentials) are presented in Fig.1. In Fig. 2 are shown the corresponding adiabatic potentials resulting from the diagonalization of $V_{vj,v'j'}(R)$. The huge difference between the diabatic and adiabatic potentials reflects the strong short-range interaction between the collisional channels, suggesting an efficient rovibrational de-excitation. The results of our preliminary close-coupling calculations confirm this expectation, in agreement with Ref. [5].

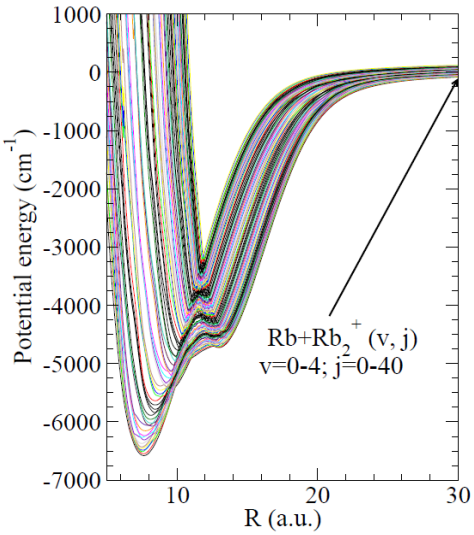

Figure 2. Rb-Rb_2^+ adiabatic potential curves.

References

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