Pathways to ultracold ground state triatomic molecules NaK_2

Baraa Shammout [1, †], **Leon Karpa** [1], **Silke Ospelkaus** [1], **Eberhard Tiemann** [1], **Olivier Dulieu** [2]

[1]Institut für Quantenoptik, Leibniz Universität Hannover, 30167 Hannover, Germany
[2]Université Paris-Saclay, CNRS, Laboratoire Aimé Cotton, Orsay, 91400, France
†corresponding author's email: shammout@iqo.uni-hannover.de

We present two theoretical approaches for forming ultracold NaK_2 triatomic molecules in its ground state. First, we propose an electric microwave association (EMWA) process [1] between ultracold K atoms and ground-state NaK molecules, relying on NaK intrinsic dipole moment and occurring below its rotational excitation energy. Using the Mapped Fourier Grid Hamiltonian method, we compute weakly bound triatomic states and association rates. Second, we investigate ro-vibronic transitions in NaK_2 between the $1^2A'$ and $3^2A'$ electronic states. From *ab initio* calculations, we obtain potential energy surfaces, transition dipole moments, and ro-vibrational energy levels using the discrete variable representation method. Based on these results, we propose a STIRAP pathway to the rovibronic ground state, using intermediate states recently observed via Feshbach-optimized photoassociation [2]. These complementary approaches offer promising routes toward creating and studying ultracold triatomic molecules.

References

[1] B. Shammout, L. Karpa, S. Ospelkaus, E. Tiemann, and O. Dulieu, *Phys. Rev. Res.* **7**, 023187 (2025).
[2] J. Cao, B.-Y. Wang, H. Yang, Z.-J. Fan, Z. Su, J. Rui, B. Zhao, and J.-W. Pan, *Phys. Rev. Lett.* **132**, 093403 (2024).