Prospects for assembling ultracold radioactive francium-silver molecules

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Molecules with unstable isotopes often contain heavy and deformed nuclei and thus possess a high sensitivity to parity-violating effects. Ultracold, micro-kelvin polar molecules with quantum-enhanced sensing capabilities can be used to measure these effects. In this presentation, I will describe our efforts to model the formation of the prototypical FrAg molecule starting from laser-cooled francium and silver atoms. In this ionically bond molecule, the parity-violating effects due to the octupole deformation of the unstable ^{223}Fr nucleus are amplified by two orders of magnitude relative to that of a spherical nucleus. This amplification is a consequence of the large electronegativity of the silver atom leading to a significant internal electric field within the molecule.

We have performed fully relativistic electronic-structure calculations of the potentials of the ground and excited states of FrAg. These calculations account for the strong spin-dependent relativistic effects of Fr and the strong ionic bond with Ag. We have also estimated the uncertainties in the ground-state potential by performing calculations with different electronic basis sets. In addition, we estimated cross sections for ultracold ^{223}Fr+^{107}Ag collisions in a magnetic field with coupled-channel calculations. These calculations led to a prediction of the nearest-neighbor densities of Fano-Feshbach resonances. These resonances can be used for magneto-association into ultracold, weakly-bound FrAg. We also determine the conditions for creating ^{223}Fr^{107}Ag molecules in their absolute ground state from these weakly-bound dimers via stimulated Raman adiabatic passage using our calculations of transition electronic dipole moments from the electronic ground to excited states. The research has been published in New Journal of Physics **24**, 025005 (2022).