Ab Initio Studies of the Collisions Involving Lanthanide Atoms and Ions

Alexei A. Buchachenko
Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Building 3 Moscow 143026 Russia
E-mail: alexei.buchachenko@gmail.com, a.buchachenko@skoltech.ru

It turns out that the bare lanthanide atoms and ions has got rapid promotion their bottom obscure period to the forefront of cold atomic and molecular physics research

Theoretical A&M physics perspectives: Sensitive probe for

Ab initio methods for interaction potentials, spin-orbit couplings, transition moments and non-adiabatic matrix elements: from 10^-6 to a few cm^-1 on energy scale

Buffer gas cooling and magnetic trapping of the Tm atom
\[ \gamma \text{ - ratio of elastic to inelastic collision rates for } M + He \text{ collisions} \]

Inelastic: transitions between Zeeman sublevels, driven by interaction anisotropy, or splitting between \( \Lambda \) (or \( \Omega \)) projections of the electronic orbital \( L \) (or total \( J \)) angular momentum on the molecular axis

\[ \text{Tm}(^4) \Rightarrow \text{TmHe} (^{2}\Sigma,^{2}\Gamma,^{2}\Delta,^{2}\Phi) \text{: ab initio SC ECP CASCF/AQCC} \]

Ab initio SC ECP CCSD(T), EOM-CCSD(T), MRCI, SI-SOCl

Yb^+ in Rb BEC: spin relaxation

Fully spin-polarized state can be created by immersing a single ion into BEC

Measurements:
- Charge transfer rate (trap “mass spectrometry”)
- Collision-induced spin relaxation (temperature and populations)

Ab initio SC ECP CCSD(T), EOM-CCSD(T), MRCI, SI-SOCl

Lanthanide dimers

Ab initio SC ECP CCSD(T) + energy differences, MRCI & AQCC

Yb_2 photoassociation in BEC

\[ \Delta D_e = 40 \text{ cm}^{-1} \]

Eu_2 in magnetic trap

Heisenberg spin coupling:
\[ J = \frac{7}{2}, S = 0 \Rightarrow 7 \]

\[ \text{E}(S) = -(7/2)(S(S+1)-s(s+1)) \]

Zeeman relaxation rate, cm^-1/s:
Heisenberg \[ 8.6 \times 10^{-13} \]

Exptl. \[ (2.5 \pm 1.5) \times 10^{-13} \]

Y. Salomonov, PASA 11, 022701 (2010)

Ion mobility: sensitivity to electronic configuration


Gd^+ (4f^75d^1, 10D), Eu^+ (4f^76s, 5S), Yb^+ (4f^146s, 5S), Lu^+ (4f^146s^2, 5S)

Ab initio SC ECP CCSD(T) + energy differences & SO MRCI

Interaction anisotropy is suppressed for submerged /shell

Yb^+ ion in Rb BEC: spin relaxation

Fully spin-polarized state can be created by immersing a single ion into BEC

Measurements:
- Charge transfer rate (trap “mass spectrometry”)
- Collision-induced spin relaxation (temperature and populations)

Ab initio SC ECP CCSD(T), EOM-CCSD(T), MRCI, SI-SOCl

Lanthanide dimers

Ab initio SC ECP CCSD(T) + energy differences, MRCI & AQCC

Yb_2 photoassociation in BEC

\[ \Delta D_e = 40 \text{ cm}^{-1} \]

Eu_2 in magnetic trap

Heisenberg spin coupling:
\[ J = \frac{7}{2}, S = 0 \Rightarrow 7 \]

\[ \text{E}(S) = -(7/2)(S(S+1)-s(s+1)) \]

Zeeman relaxation rate, cm^-1/s:
Heisenberg \[ 8.6 \times 10^{-13} \]

Exptl. \[ (2.5 \pm 1.5) \times 10^{-13} \]

Y. Salomonov, PASA 11, 022701 (2010)