Multi-Channel Scattering Calculation for Ultracold Ion-Atom Collisions

Competing excitation quenching and charge exchange in ultracold Li-Ba^+ collisions

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Andrea Orbán and **Olivier Dulieu**

collaboration with University of Freiburg

Introduction

- <u>Ultracold</u> <u>quantum</u> gases (e.g. atoms, molecules, ions, ...)

↓

1 μK – 1 nK

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- atom – ion mixed system in hybrid traps

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- dilute gases ⟶ long-range interactions relevant: atom-ion $\sim \frac{1}{R^4}$
  ($10^8 – 10^{13}$ atom/cm^3)

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- atom – ion mixed system in hybrid traps

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- application: precision measurements,
  quantum controlled chemistry,
  quantum technology, ...

Introduction

- The project focuses on the **theoretical modelling** of the dynamics of **ion-neutral systems at ultracold temperatures** in order to design ways for their full quantum control

- Our aims are connected to **ongoing** cutting-edge experimental investigations with hybrid traps (Uni. Freiburg, Weizmann Inst., Uni. Basel, Uni. Ulm, Uni. Osaka, Uni. Hannover)

- Understanding ion-neutral ultracold collisions

Introduction

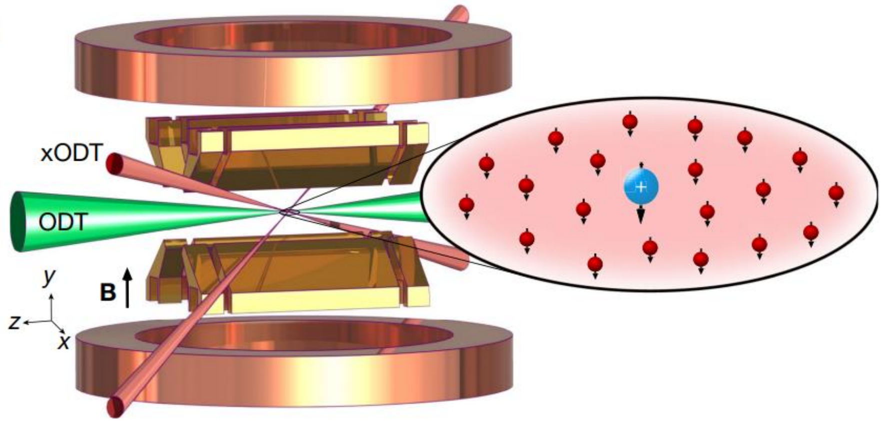
- Understanding such ultracold collisions relies on the combination of various expertise:
  - perform detailed atomic and molecular structure calculations
  - determine electronically excited molecular states generated by lasers in experiments
  - perform dynamical calculations based on the quantum coupled-channel description of the collision including both long-range (electrostatic) and short-range (chemical) interactions

- These methodologies will be applied to two species of atom-ion pairs of relevance for ongoing experiments:

^{6}Li - $^{138}Ba^{+}$, in collab. with Uni. Freiburg
^{87}Rb - $^{88}Sr^{+}$, in collab. with Weizmann Inst.

Preparation

Experiment: Uni. Freiburg



P. Weckesser et. al, Nature, 600:429, 2021

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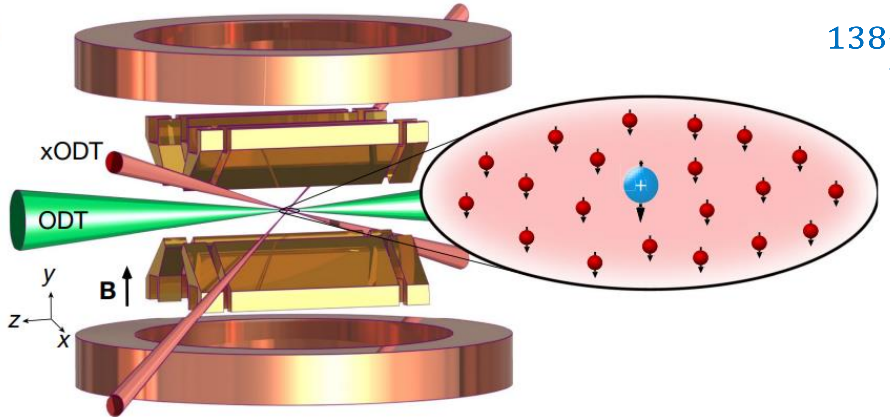

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$^{138}\mathbf{Ba}^{+}$: single ion

$\sim 365\ \mu K$ in the lab

metastable $5D_{5/2,3/2}$ excited state
(lifetime 32 s, 80 s)

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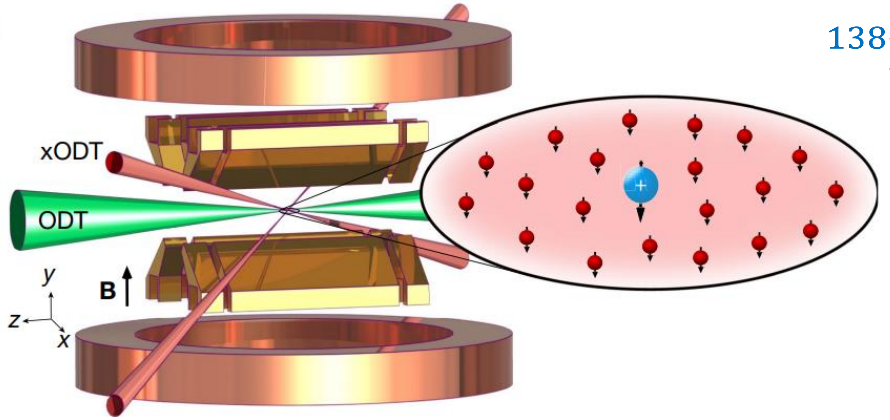

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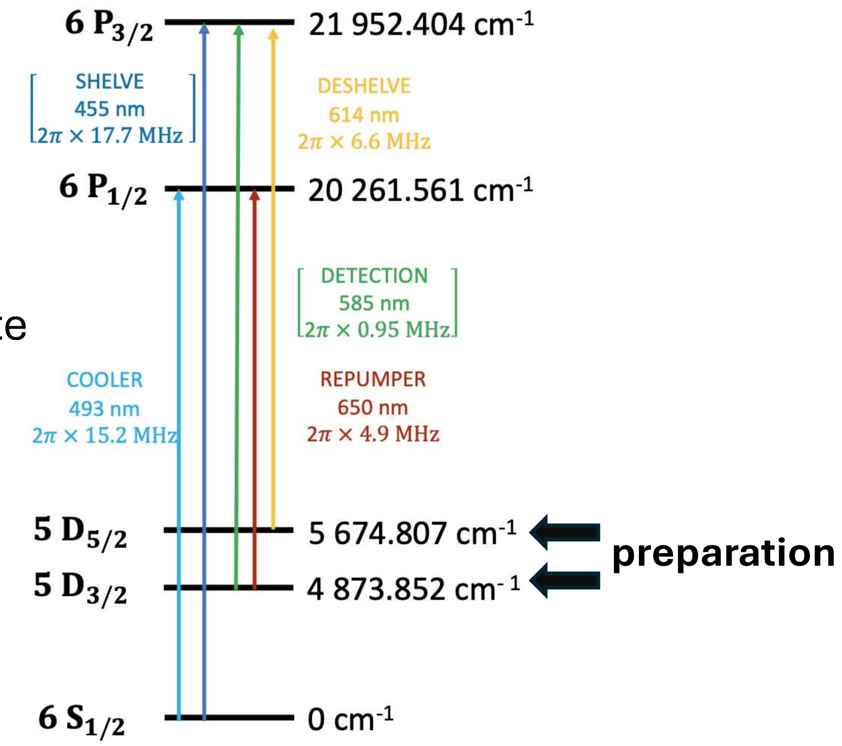

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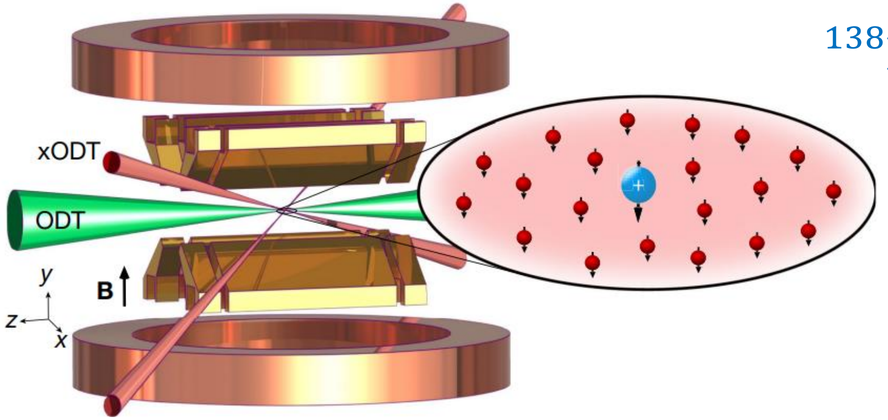

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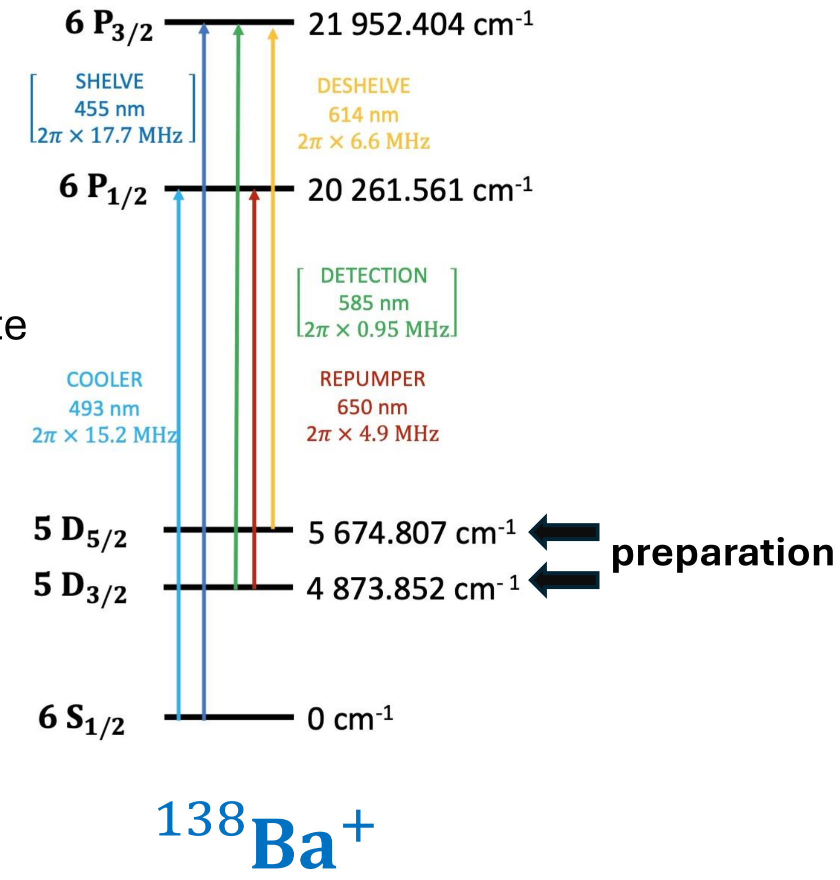
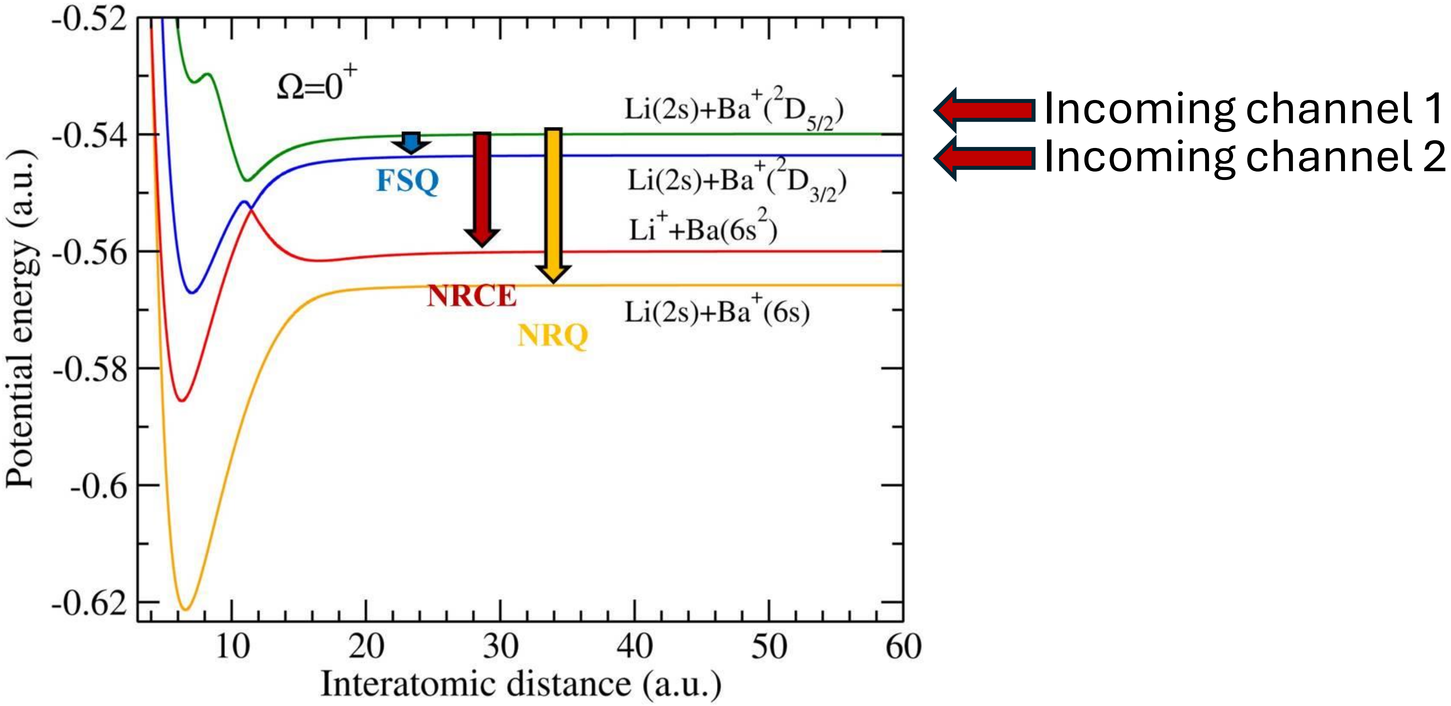
$^{6}\mathbf{Li}$: $1-3\ \mu K$ in the lab

$2S_{1/2}$ ground state

few thousand atom
close to quantum degeneracy



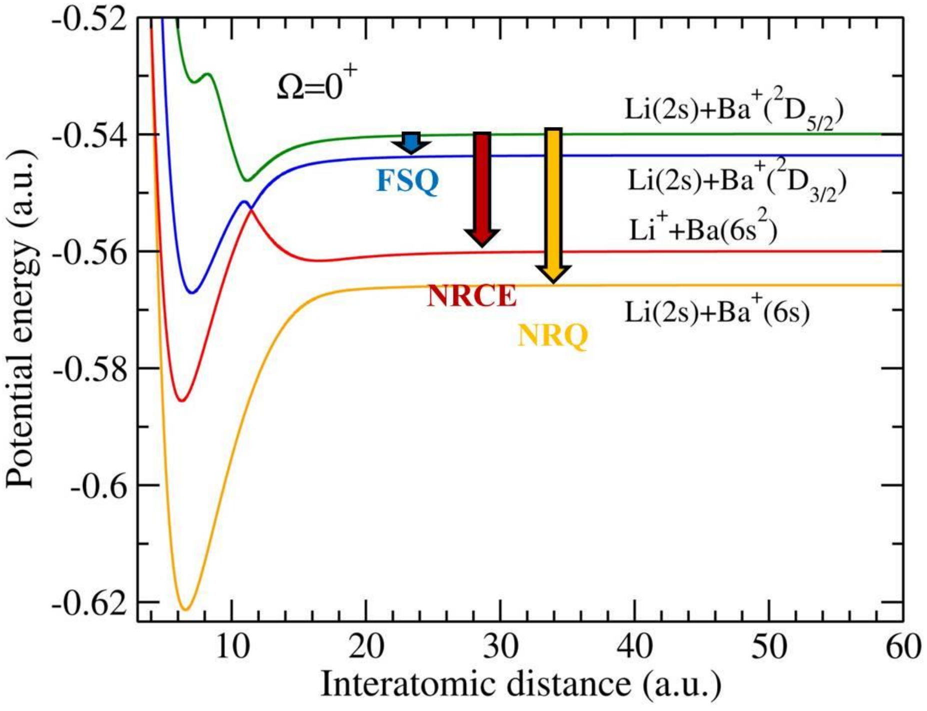
Observed processes



Purpose: theoretical description of the observed processes

Molecular structure calculated by THEOMOL group

Observed processes



Incoming channel 1
Incoming channel 2

- FSQ (Fine Structure Quenching)

  $Li(2S_{1/2}) + Ba^{+}(5D_{5/2}) \rightarrow$
  $\rightarrow (2S_{1/2}) + Ba^{+}(5D_{3/2})$

- NRCE (Non-Radiative Charge Exchange)

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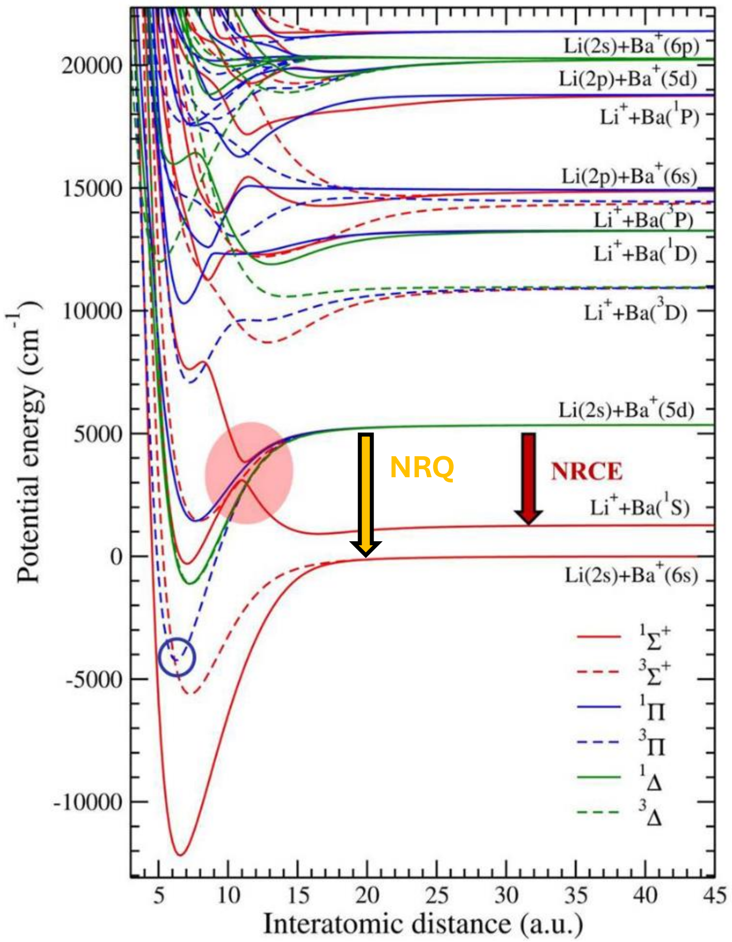
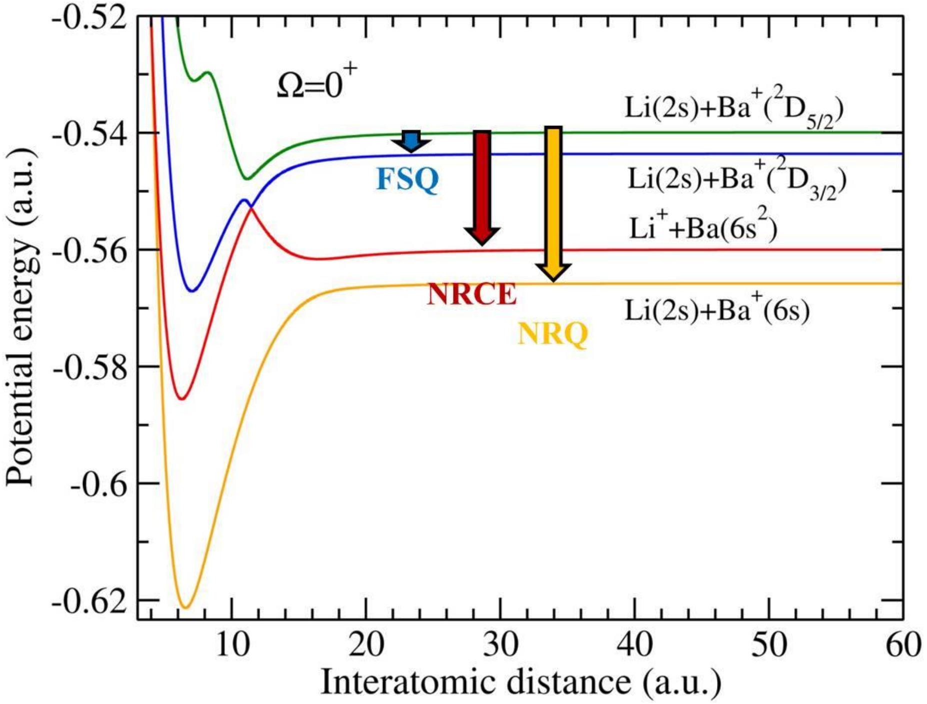
Hund's case a)





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Potential energy in the molecular frame

$$\boldsymbol{H}(R) = -\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2} + \underbrace{V(R) + V_{SOC}(R)}$$

16×16

	$\Omega=0^+$				$\Omega=0^-$			$\Omega=1$					$\Omega=2$			$\Omega=3$
	S+S	Ion+S	S+D		S+S	S+D		S+S	S+D				S+D			S+D
	$1\,^1\Sigma^+$	$2\,^1\Sigma^+$	$3\,^1\Sigma^+$	$1\,^3\Pi$	$1\,^3\Sigma^+$	$2\,^3\Sigma^+$	$1\,^3\Pi$	$1\,^3\Sigma^+$	$2\,^3\Sigma^+$	$1\,^1\Pi$	$1\,^3\Pi$	$1\,^3\Delta$	$1\,^3\Pi$	$1\,^1\Delta$	$1\,^3\Delta$	$1\,^3\Delta$
$1\,^1\Sigma^+$	$V(1\,^1\Sigma^+)$	0	0	$A_{1,4}$												
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$1\,^3\Sigma^+$								$V(1\,^3\Sigma^+)$	0	$A_{8,10}$	$A_{8,11}$	0				
$2\,^3\Sigma^+$								0	$V(2\,^3\Sigma^+)$	$A_{9,10}$	$A_{9,11}$	0				
$1\,^1\Pi$								$A_{10,8}$	$A_{10,9}$	$V(1\,^1\Pi)$	$A_{10,11}$	$A_{10,12}$				
$1\,^3\Pi$								$A_{11,8}$	$A_{11,9}$	$A_{11,10}$	$V(1\,^3\Pi)$	$A_{11,12}$				
$1\,^3\Delta$								0	0	$A_{12,10}$	$A_{12,11}$	$V(1\,^3\Delta)$ $+A_{12,12}$				
$1\,^3\Pi$													$V(1\,^3\Pi)$ $+A_{13,13}$	$A_{13,14}$	$A_{13,15}$	
$1\,^1\Delta$													$A_{14,13}$	$V(1\,^1\Delta)$	$A_{14,15}$	
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$V(\ldots)$ – Hund's case a) potential energy curves

$A_{i,j}$ – spin – orbit coupling matrix element

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Diagonalization

Hund's case c) potential energy curves

Frame transformation

coordinate system transformation

Molecular frame

$\{\ |\Lambda, S, \Sigma, \Omega = \Lambda + \Sigma, J, parity\rangle\ \}$

→

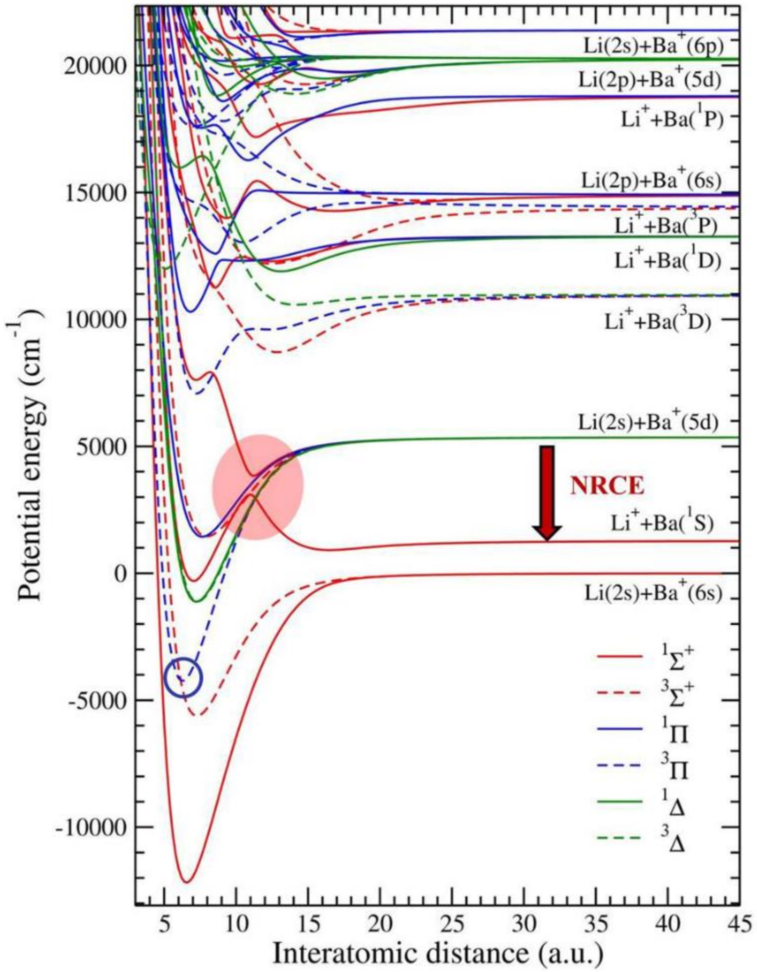
Laboratory frame

$\{\ |j_A, j_B, j, l, J, parity\rangle\ \}$

Molecular structure

Molecular frame

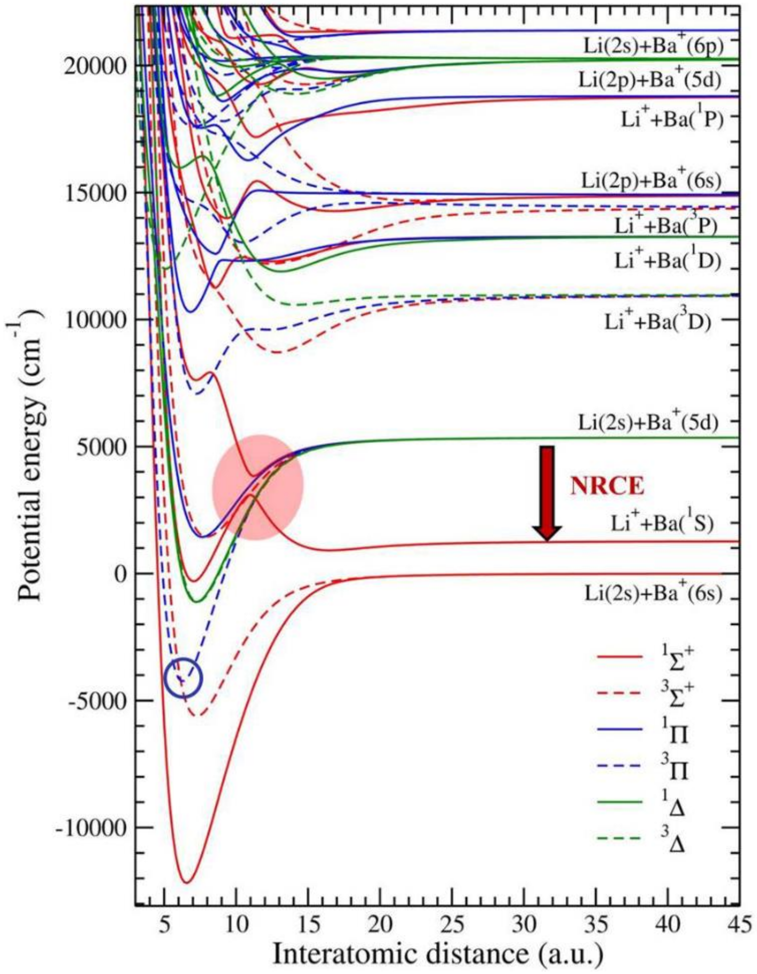
Hund's case a)



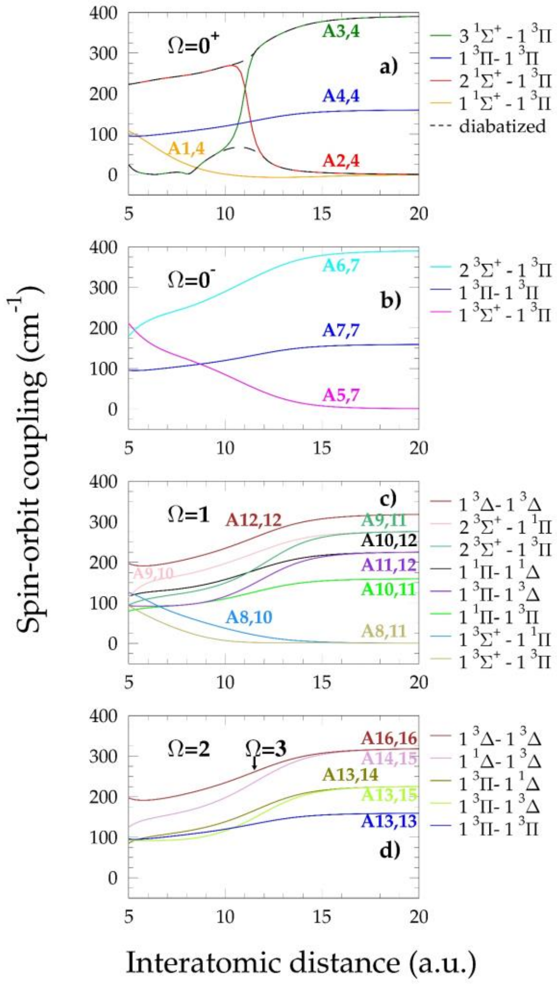
Molecular structure

Molecular frame

Hund's case a)



Spin – orbit coupling



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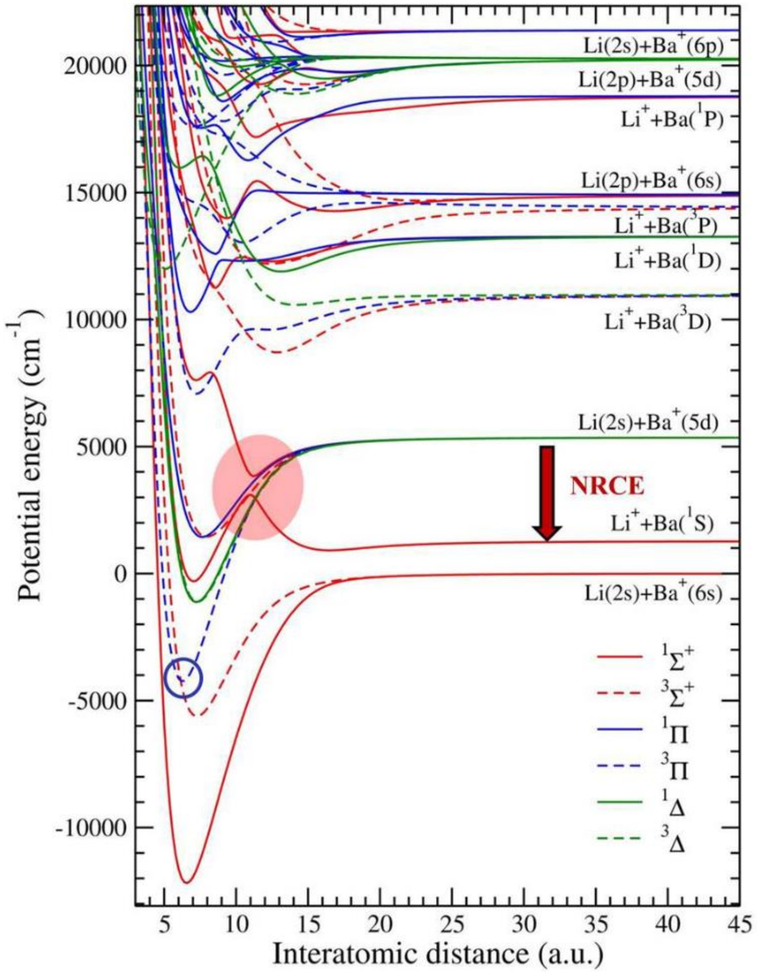

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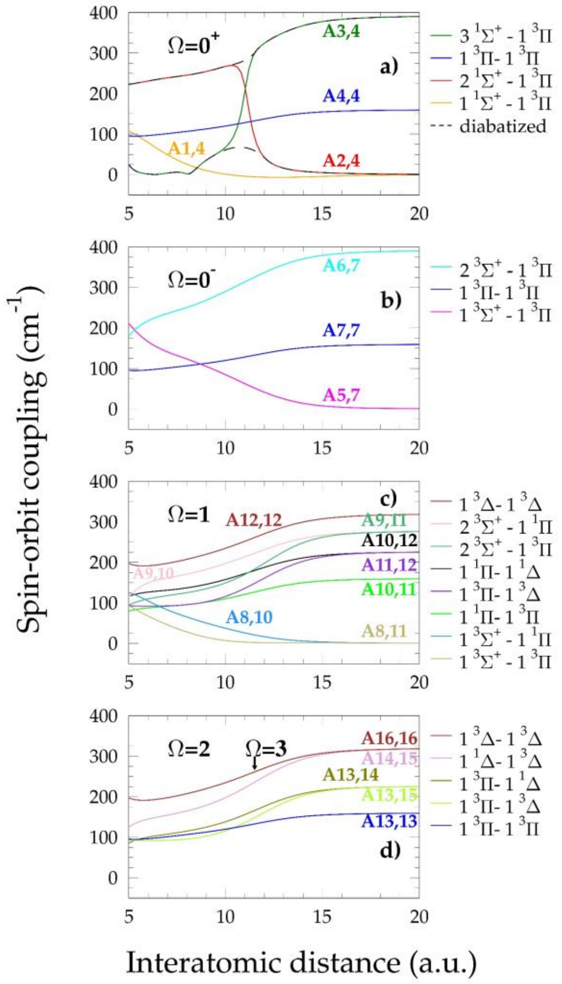

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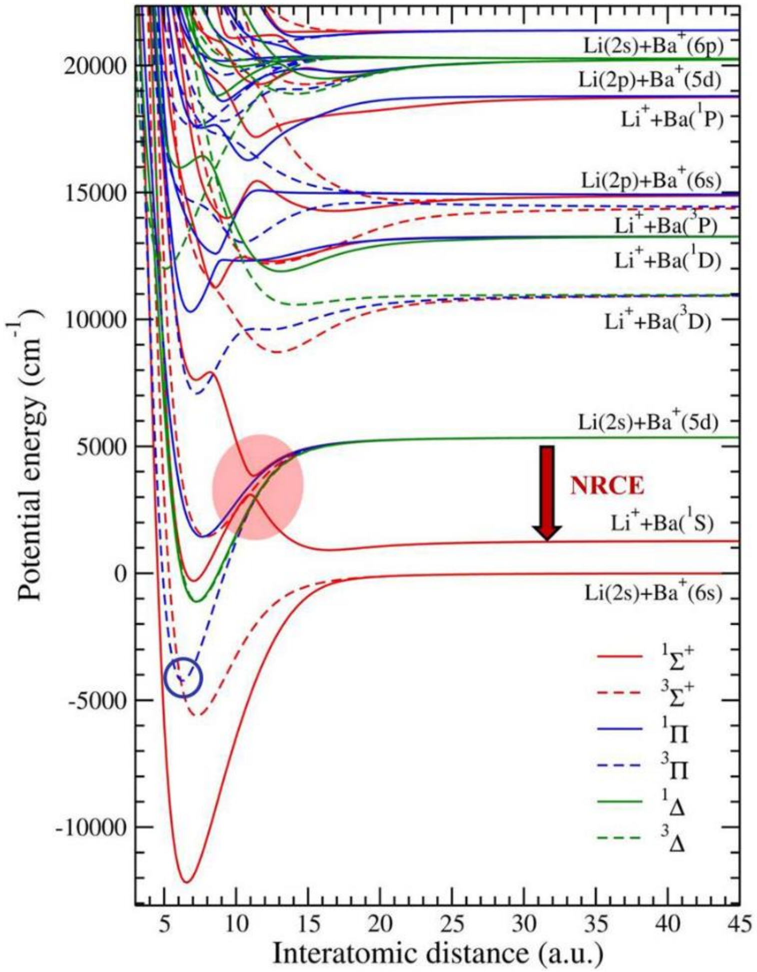
Transformation

Molecular structure

Molecular frame → **Laboratory frame**

Hund's case a)



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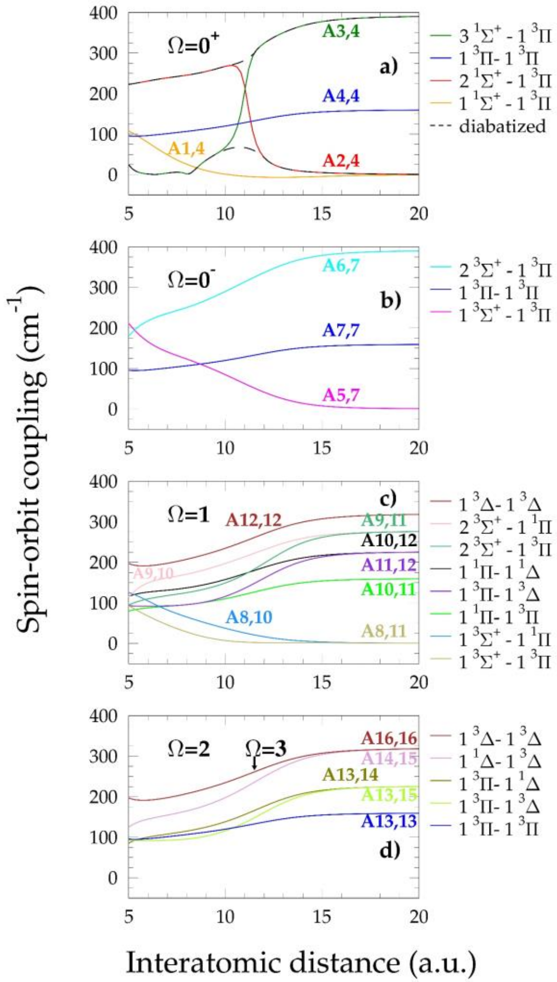


+

Transformation

=

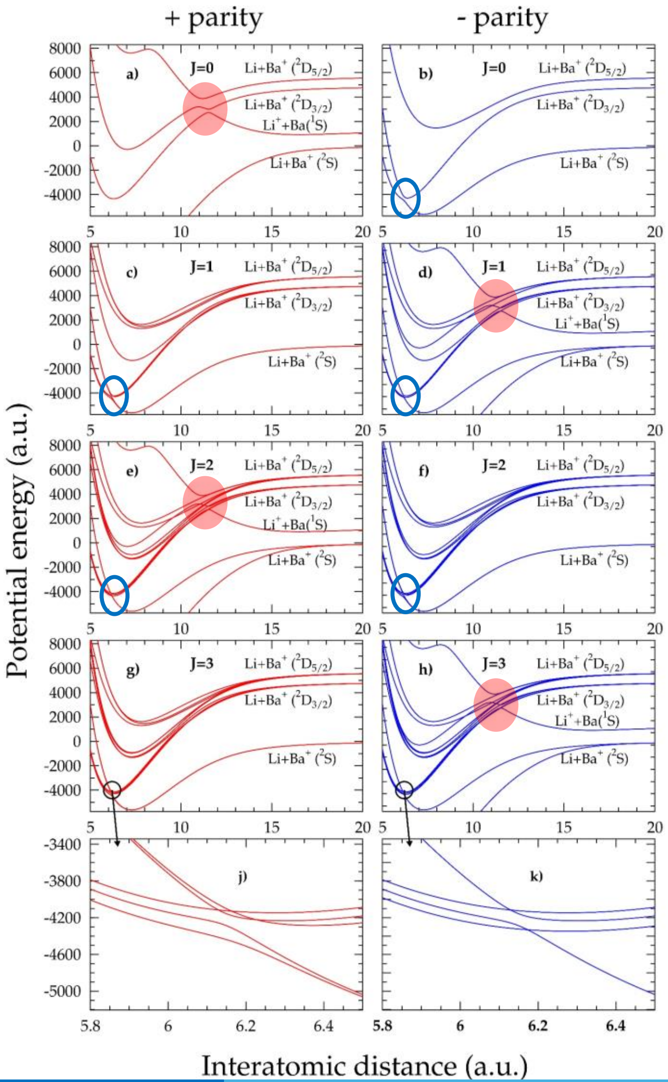
J = 0

J = 1

J = 2

J = 3

Hund's case e)



Multi-Channel Quantum Scattering (MCQS)

Cross section

$$\boldsymbol{\sigma}_{i\to f}(E) = \frac{\pi}{k_0^2}\sum_J (2J+1) \sum_{\substack{l_i, j_i, m_i \\ l_f, j_f, m_f}} \left| \boldsymbol{\mathcal{S}}\left(J, l_f, j_f, m_f, p \leftarrow J, l_i, j_i, m_i, p\right) \right|^2$$

where, $\mathcal{S}$ – S – matrix
J – total angular momentum quantum number
l – partial wave
j – electronic angular momentum quantum number
m – projectile of the electronic angular momentum
p – parity

Rate $\boldsymbol{K}(E) = \left(\frac{2E}{\mu}\right)^{\frac{1}{2}} \boldsymbol{\sigma}_{i\to f}(E)$

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Hamiltonian

$$\boldsymbol{H}_l(R) = -\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2}\boldsymbol{I} + \frac{\hbar^2(l(l+1)}{2\mu R^2}\boldsymbol{I} + \boldsymbol{V}(R) + \boldsymbol{V}_{SOC}(R)$$

where, μ reduced mass
- $\boldsymbol{I}$ – identity matrix
- $\boldsymbol{V}(R)$ - electronic potential energy matrix
- $\boldsymbol{V}_{SOC}(R)$ – spin – orbit matrix
- l – partial wave

Scattered wave function for the α- channel

$$\psi_\alpha(R) = R^{-1}\sum_i \phi_i(\tau)F_{i\alpha}(R)$$

where, $\phi_i(\tau)$ – orthonormal basis
- τ – atom/ion all quantum number configuration
- $F_{i\alpha}(R)$ – radial channel function

Coupled equations for $F_{j\alpha}(R)$

$$\frac{d^2F_{j\alpha}(R)}{dr^2} = \sum_i [W_{ij} - E\delta_{ij}]F_{i\alpha}(R)$$

where, $W_{ij} = \frac{2\mu}{\hbar^2}\int \phi_j^*(\tau)\left[V_{SOC} + V(R) + \frac{\hbar^2(l(l+1)}{2\mu R^2}\right]\phi_i(\tau)d\tau$

Competing processes

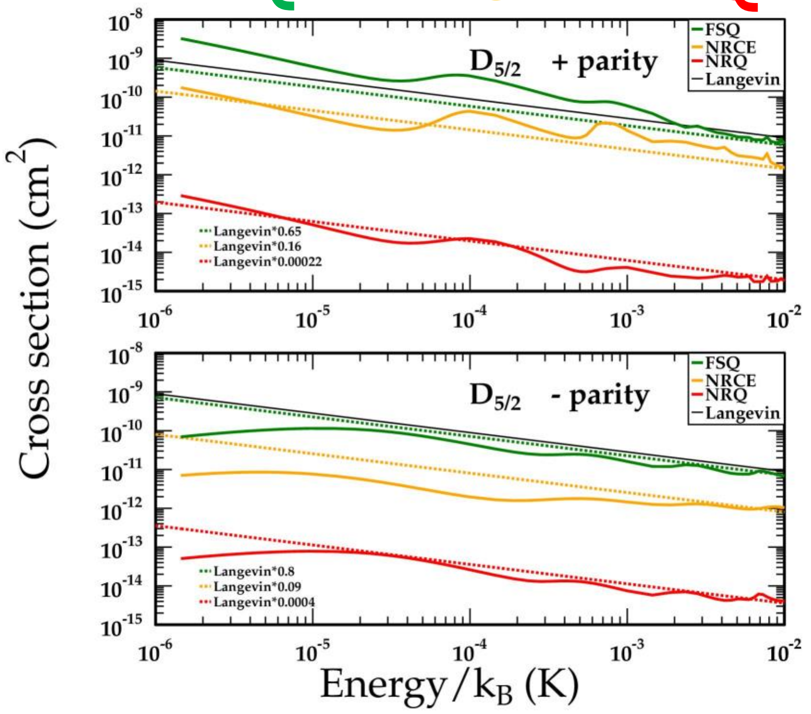
- FSQ (Fine Structure Quenching)
- NRCE (Non-Radiative Charge Exchange)
- NRQ (Non-Radiative Quenching)

Incoming channel

$Li(2S_{1/2})$ + Ba^+(**$5D_{5/2}$**)

Cross section

FSQ NRCE NRQ



https://arxiv.org/abs/2406.16017

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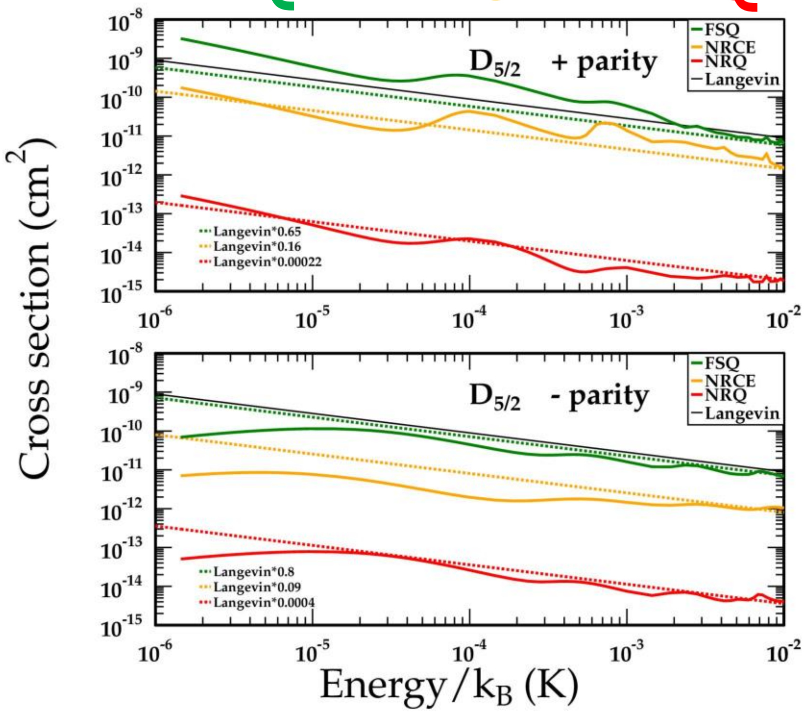
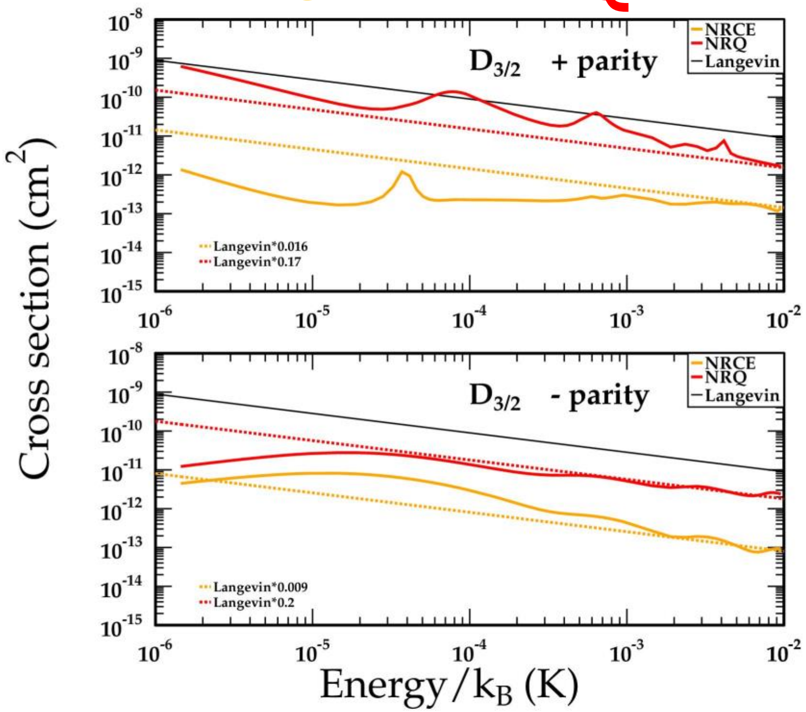
Incoming channel

$Li(2S_{1/2})$ + Ba$^+$(**5D$_{5/2}$**) $Li(2S_{1/2})$ + Ba$^+$(**5D$_{3/2}$**)

Cross section

FSQ NRCE NRQ **NRCE NRQ**





https://arxiv.org/abs/2406.16017

Competing processes

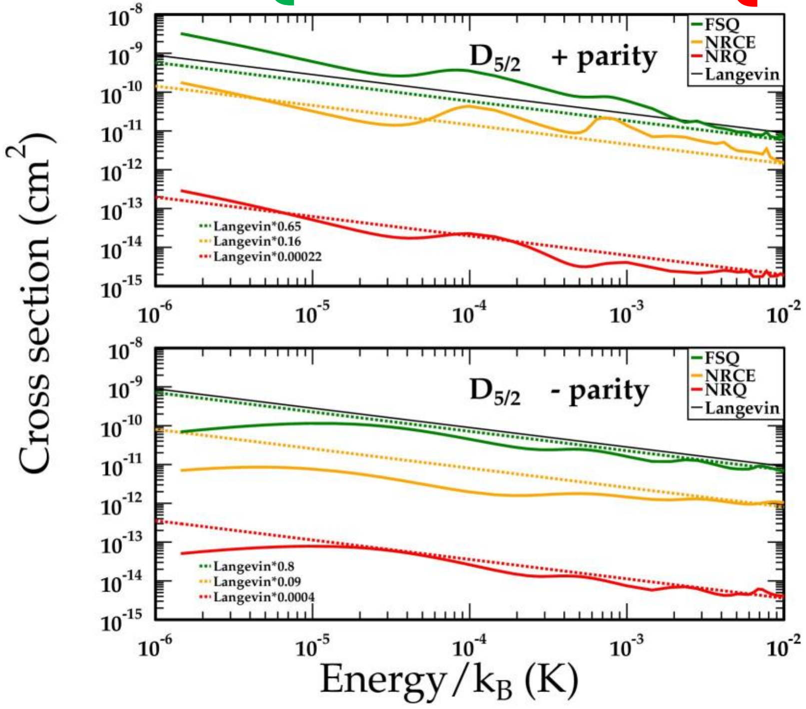
- FSQ (Fine Structure Quenching)
- NRCE (Non-Radiative Charge Exchange)
- NRQ (Non-Radiative Quenching)

Incoming channel

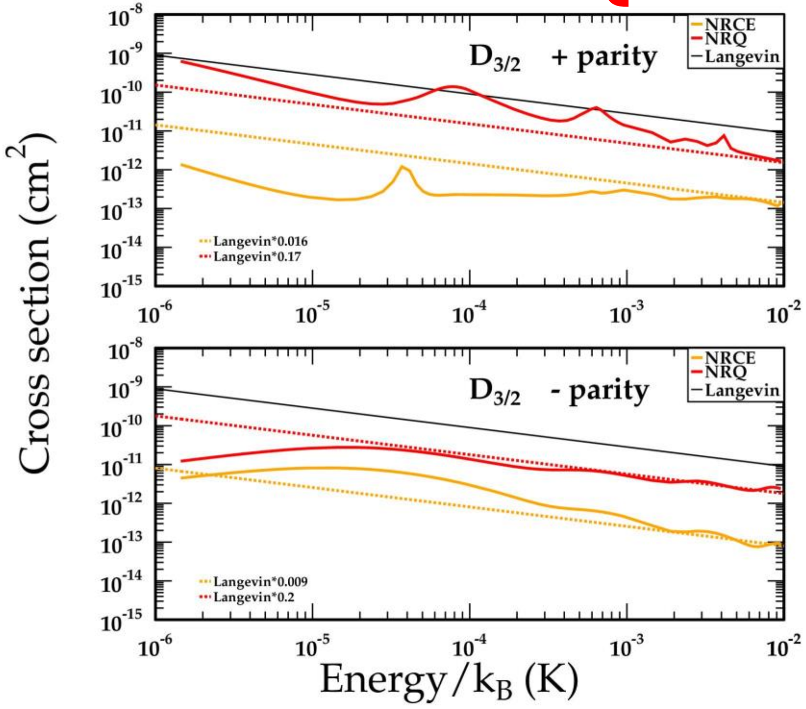
Li($2S_{1/2}$) + Ba^{+}(**5D$_{5/2}$**) Li($2S_{1/2}$) + Ba^{+}(**5D$_{3/2}$**)

Cross section

FSQ NRCE NRQ



NRCE NRQ



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Langevin cross section:

$$\sigma_L = 2\pi\sqrt{\frac{\alpha}{2E}},$$

α – polarizability of the atom

E – collisional energy

Competing processes

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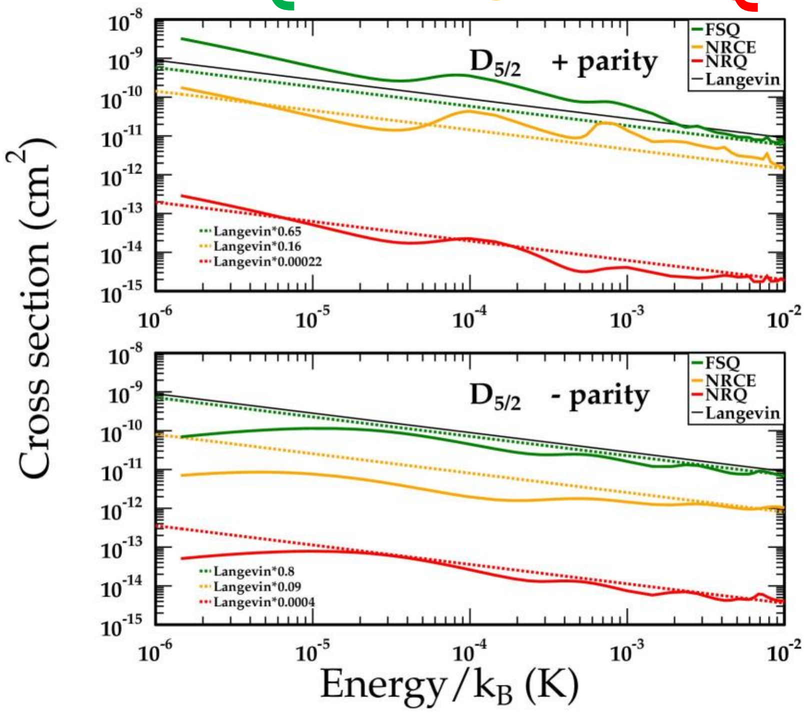
Incoming channel

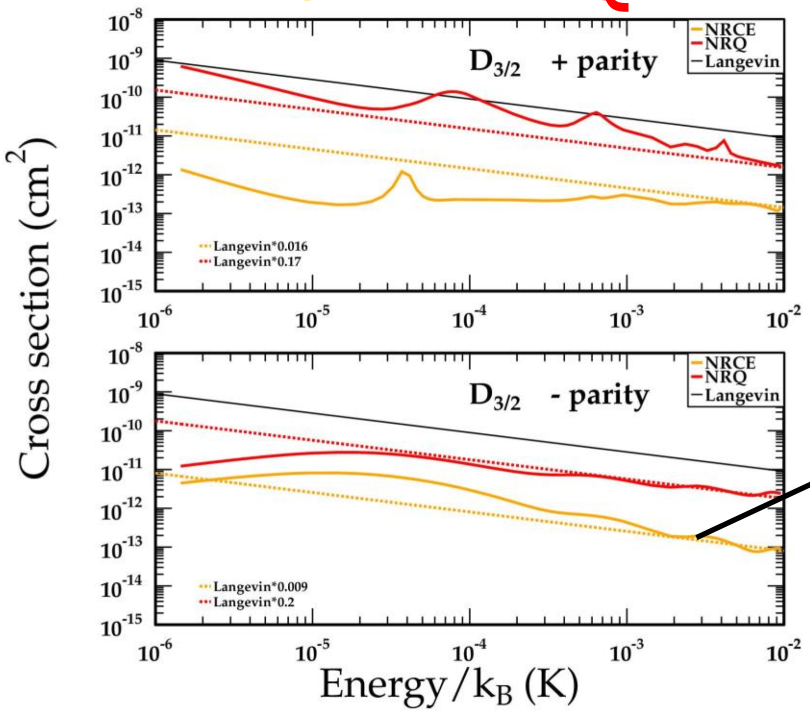
$\mathrm{Li}(2S_{1/2}) + \mathrm{Ba}^{+}(\mathbf{5D_{5/2}})$ $\mathrm{Li}(2S_{1/2}) + \mathrm{Ba}^{+}(\mathbf{5D_{3/2}})$

Cross section

FSQ **NRCE** **NRQ**

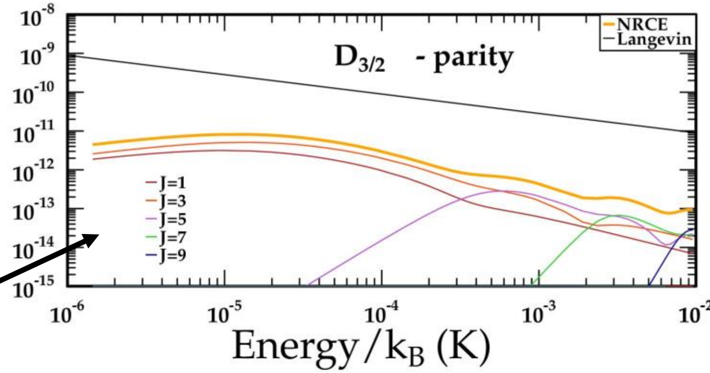


NRCE **NRQ**



Partial cross section

NRCE



Langevin cross section:

$\sigma_L = 2\pi\sqrt{\frac{\alpha}{2E}},$ α – polarizability of the atom

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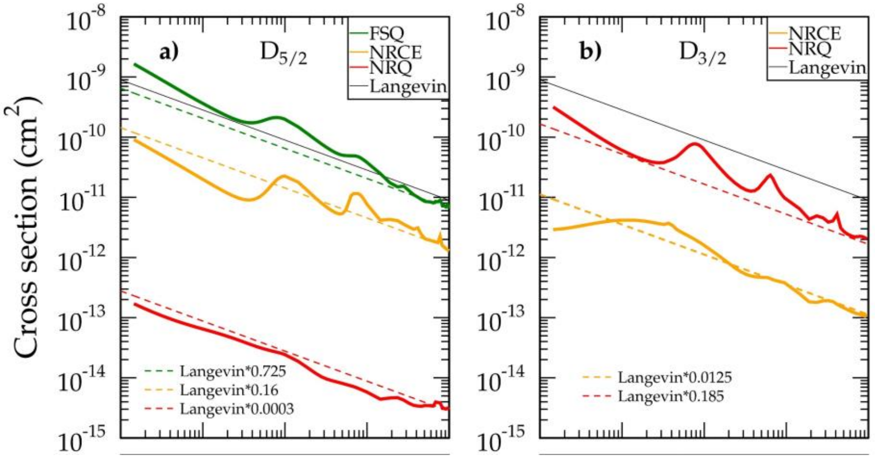
Cross sections and reaction rates

- FSQ (Fine Structure Quenching)
- NRCE (Non-Radiative Charge Exchange)
- NRQ (Non-Radiative Quenching)

Cross section



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Cross sections and reaction rates

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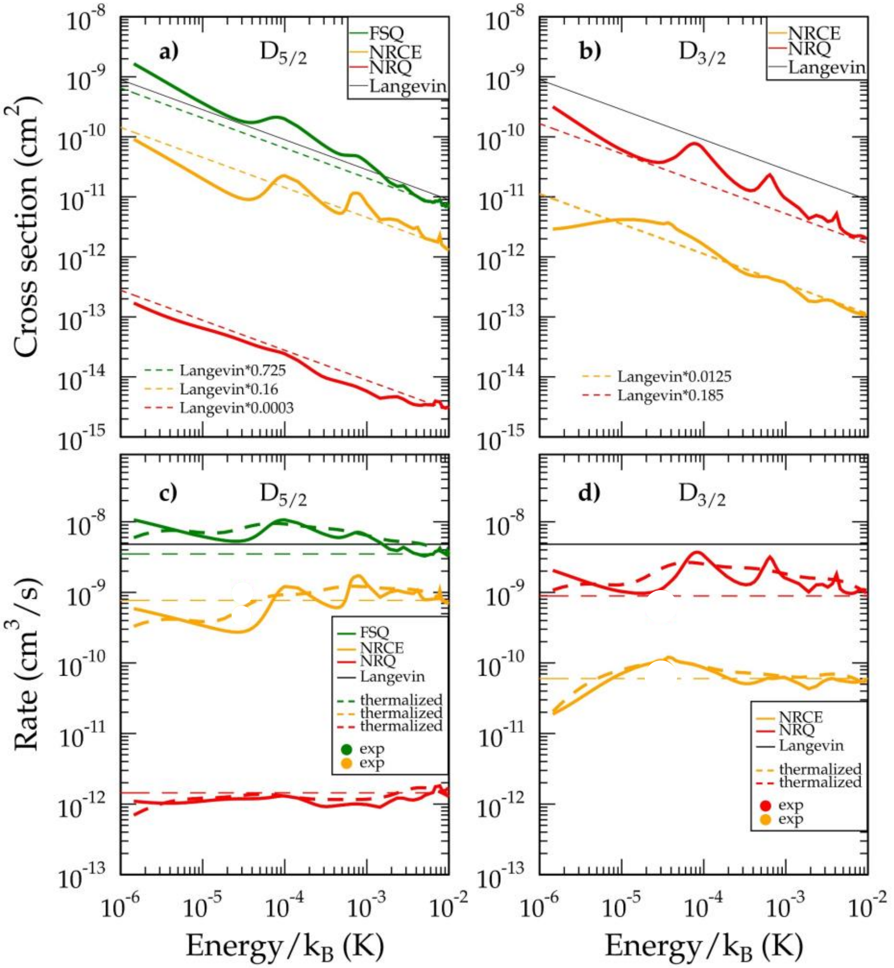
Cross section



Rate

https://arxiv.org/abs/2406.16017

Cross sections and reaction rates

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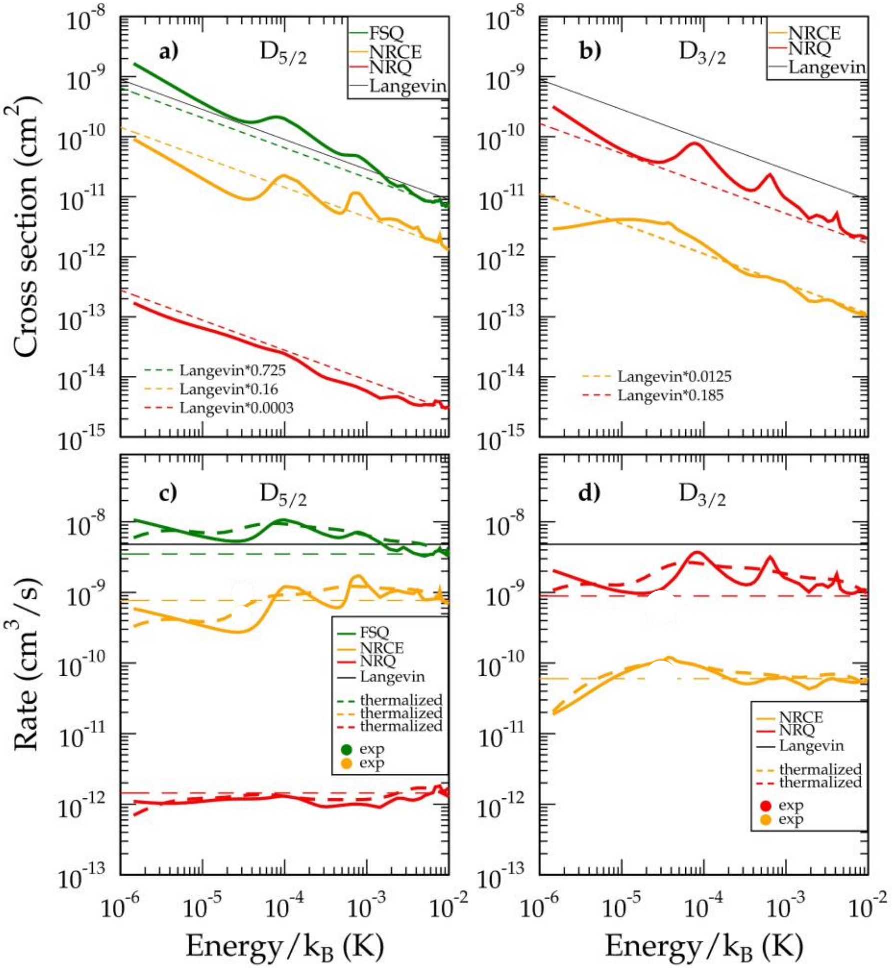
Cross section



Rate

THEO.

$D_{3/2}$:

$\text{Rate}_{\text{NRCE}} < \text{Rate}_{\text{NRQ}}$

$D_{5/2}$:

$\text{Rate}_{\text{NRCE}} > \text{Rate}_{\text{NRQ}}$

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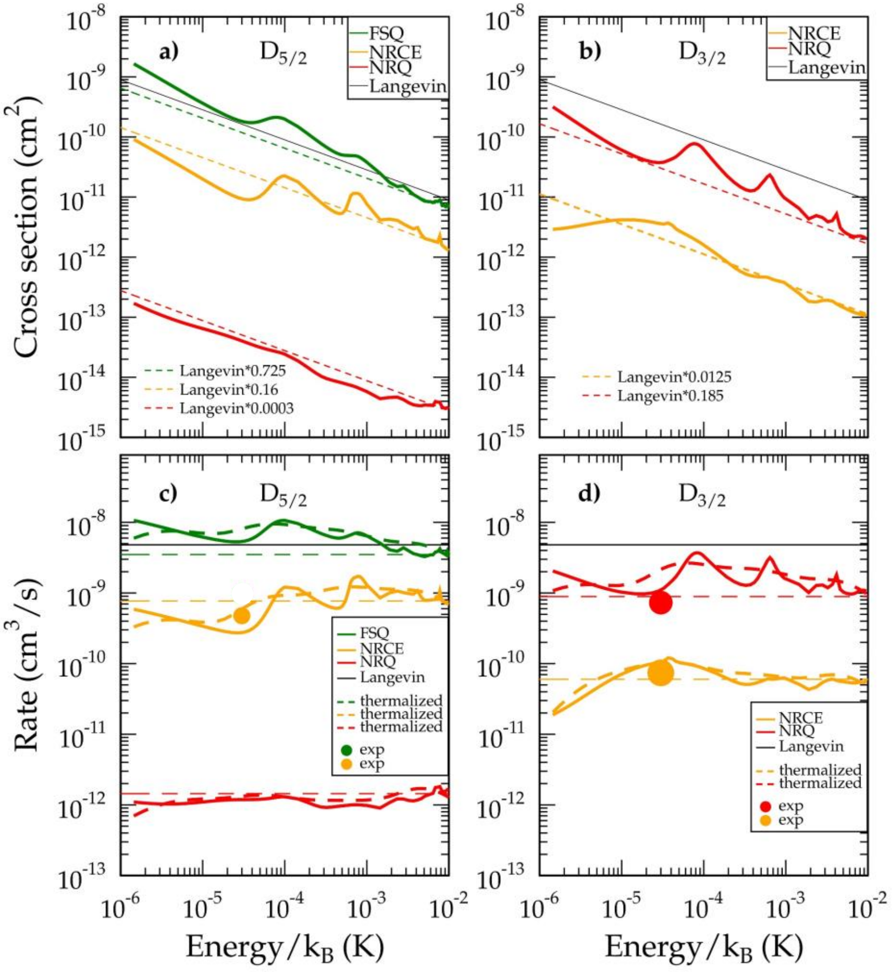
Cross sections and reaction rates + experiment

- FSQ (Fine Structure Quenching)
- NRCE (Non-Radiative Charge Exchange)
- NRQ (Non-Radiative Quenching)

Cross section



Rate

	THEO.	**EXP.**
$D_{3/2}$:	$\text{Rate}_{\text{NRCE}} < \text{Rate}_{\text{NRQ}}$	✔
$D_{5/2}$:	$\text{Rate}_{\text{NRCE}} > \text{Rate}_{\text{NRQ}}$	✔

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Cross sections and reaction rates + experiment

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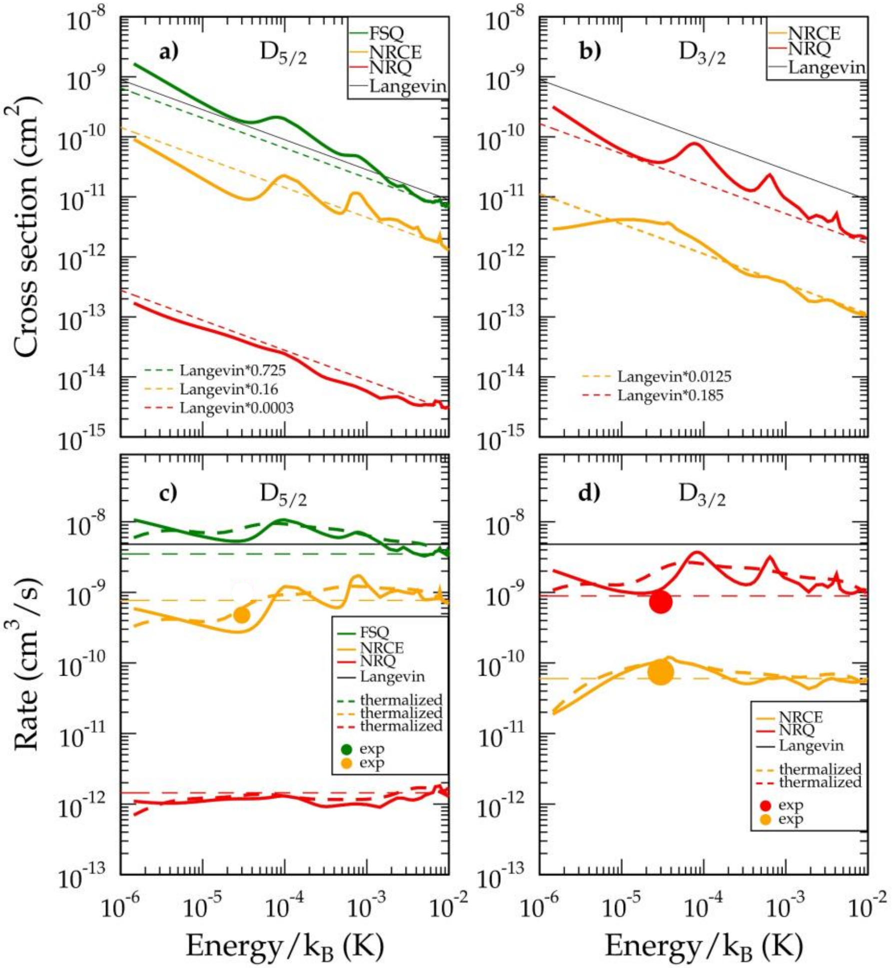
- NRCE (Non-Radiative Charge Exchange)
- NRQ (Non-Radiative Quenching)

Cross section



Rate

	THEO.	**EXP.**
$D_{3/2}$:	$Rate_{NRCE} < Rate_{NRQ}$	✔
$D_{5/2}$:	$Rate_{NRCE} > Rate_{NRQ}$	✔

THEO.

$Rate_{FSQ} > Rate_{NRCE}$

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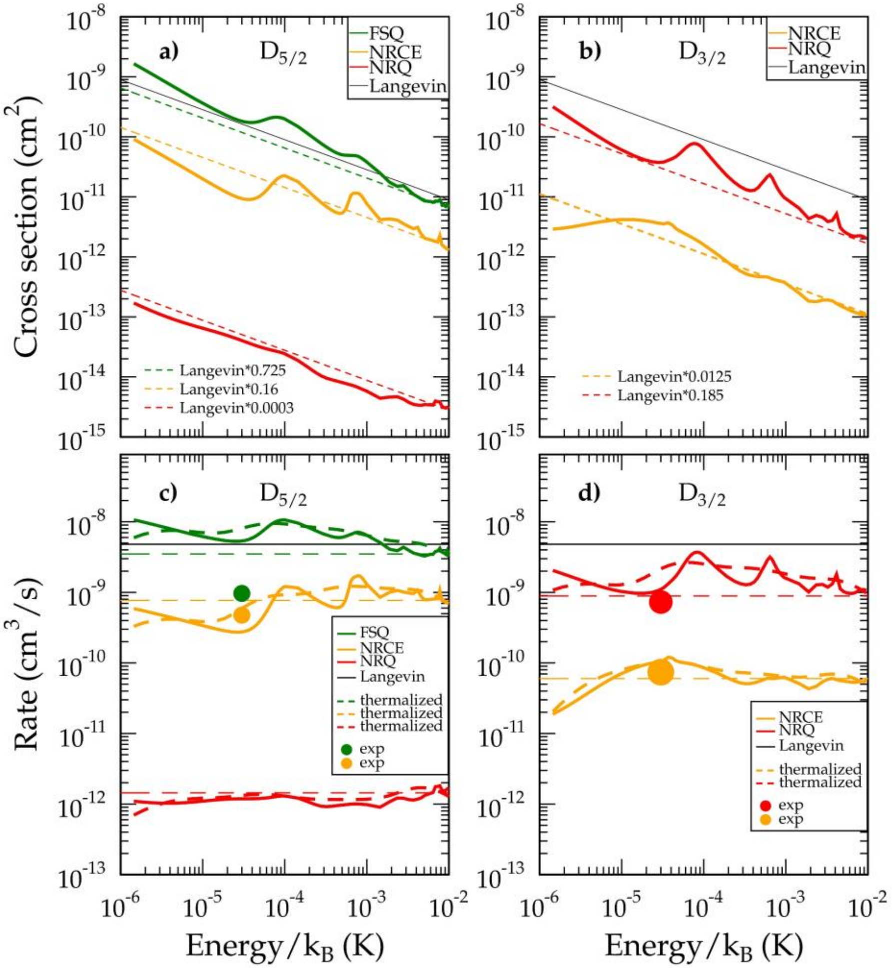
Cross sections and reaction rates + experiment

- FSQ (Fine Structure Quenching)
- NRCE (Non-Radiative Charge Exchange)
- NRQ (Non-Radiative Quenching)

Cross section



Rate

	THEO.	EXP.	THEO.	EXP.
$D_{3/2}$:	$Rate_{NRCE} < Rate_{NRQ}$	✔		
$D_{5/2}$:	$Rate_{NRCE} > Rate_{NRQ}$	✔	$Rate_{FSQ} > Rate_{NRCE}$	✔

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Cross sections and reaction rates + experiment

- FSQ (Fine Structure Quenching)
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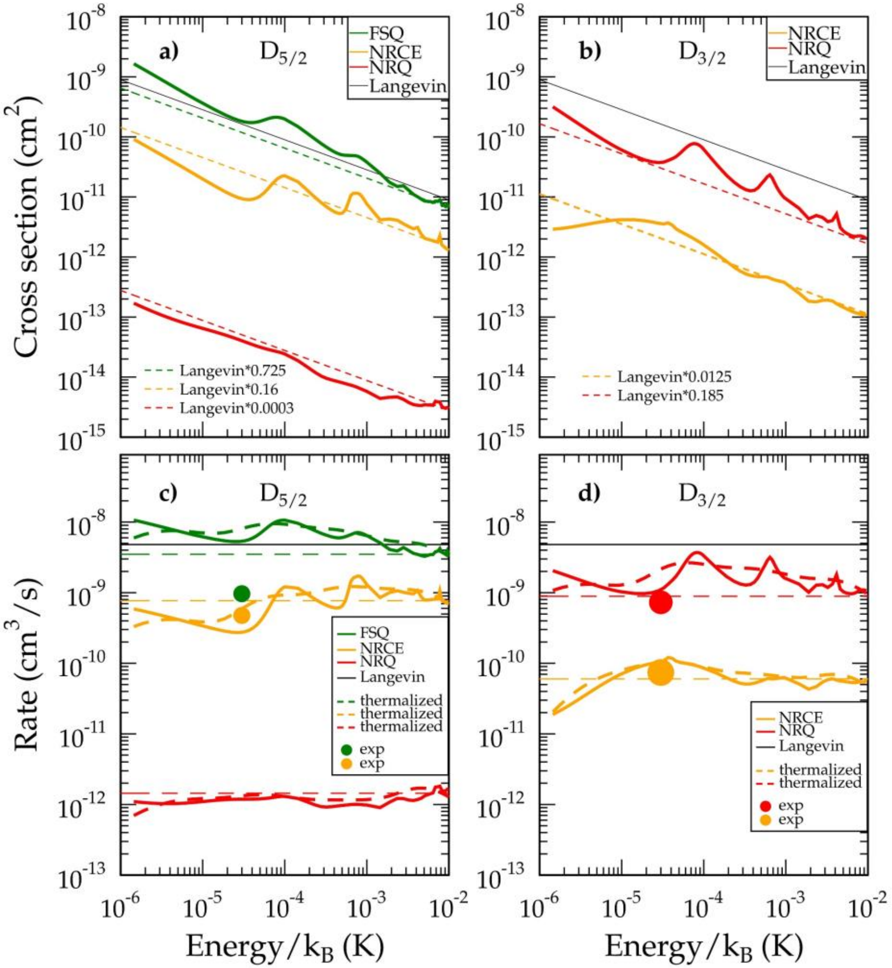
Cross section



Rate

	THEO.	EXP.	THEO.	EXP.
$D_{3/2}$:	$Rate_{NRCE} < Rate_{NRQ}$	✓		
$D_{5/2}$:	$Rate_{NRCE} > Rate_{NRQ}$	✓	$Rate_{FSQ} > Rate_{NRCE}$	✓

Good agreement with the experiment!

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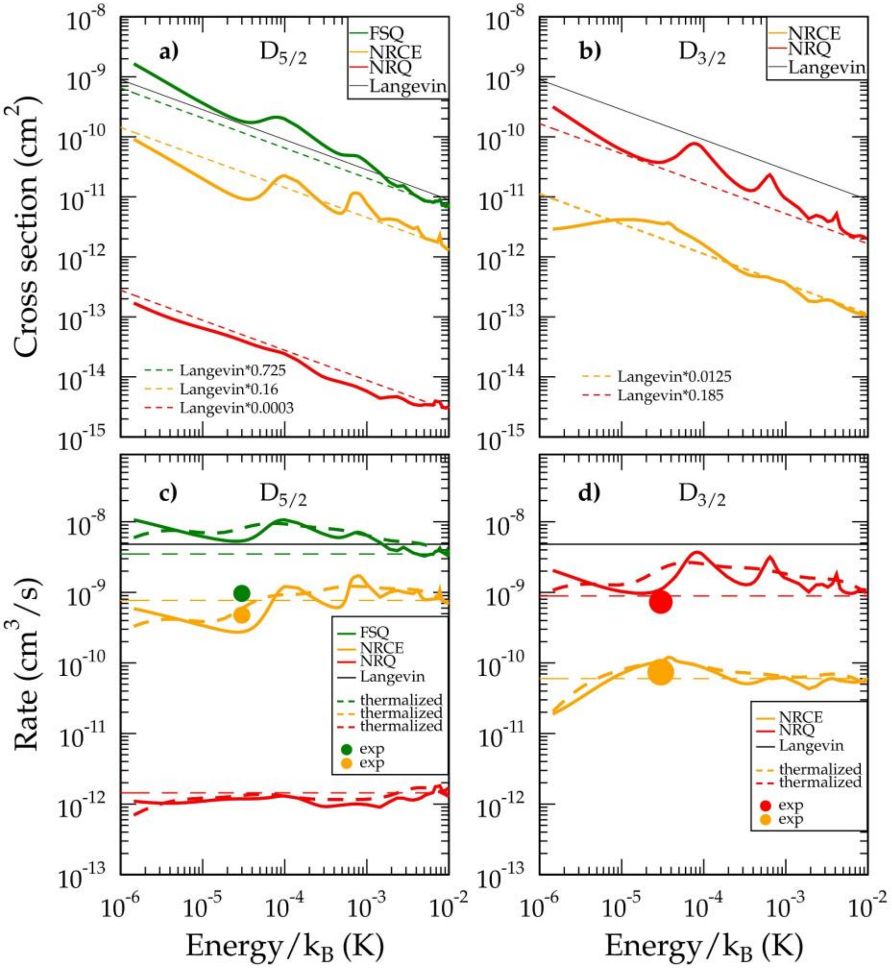
Cross sections and reaction rates + experiment

- FSQ (Fine Structure Quenching)
- NRCE (Non-Radiative Charge Exchange)
- NRQ (Non-Radiative Quenching)

Cross section



Rate

	THEO.	EXP.	THEO.	EXP.
$D_{3/2}$:	$\text{Rate}_{\text{NRCE}} < \text{Rate}_{\text{NRQ}}$	✔		
$D_{5/2}$:	$\text{Rate}_{\text{NRCE}} > \text{Rate}_{\text{NRQ}}$	✔	$\text{Rate}_{\text{FSQ}} > \text{Rate}_{\text{NRCE}}$	✔

$D_{3/2}$:

$$\frac{\text{Rate}_{\text{NRQ}}}{\text{Rate}_{\text{NRCE}}} \approx 10$$

$D_{5/2}$:

$$\frac{\text{Rate}_{\text{NRQ}}}{\text{Rate}_{\text{NRCE}}} \approx 0.001 \qquad \frac{\text{Rate}_{\text{FSQ}}}{\text{Rate}_{\text{NRCE}}} \approx 10 \qquad \frac{\text{Rate}_{\text{FSQ}}}{\text{Rate}_{\text{NRQ}}} \approx 10^4$$

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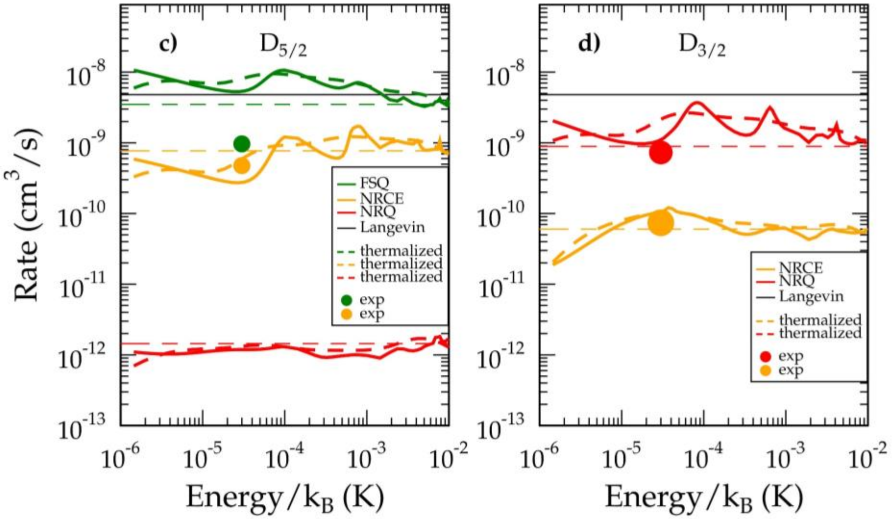
Summary



- Good agreement between the theory and experiment for the NRCE process

- For $D_{3/2}$ incoming channel the theory predicts that the NRQ process has higher probability than the NRCE, which is consistent with the experiment

- For $D_{5/2}$ incoming channel they could not detect NRQ in the experiment, our theory can confirm that, it predicts such a low probability

- For $D_{5/2}$ incoming channel the theory overestimates the FSQ process, which could be explained by unaccurate spin – orbit coupling determination → clarification needed

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Outlook and perspectives

- Similar investigations for the same class of systems (eg. Rb - Sr^+)
  - different observed process (**electronic excitation exchange, EEE**)

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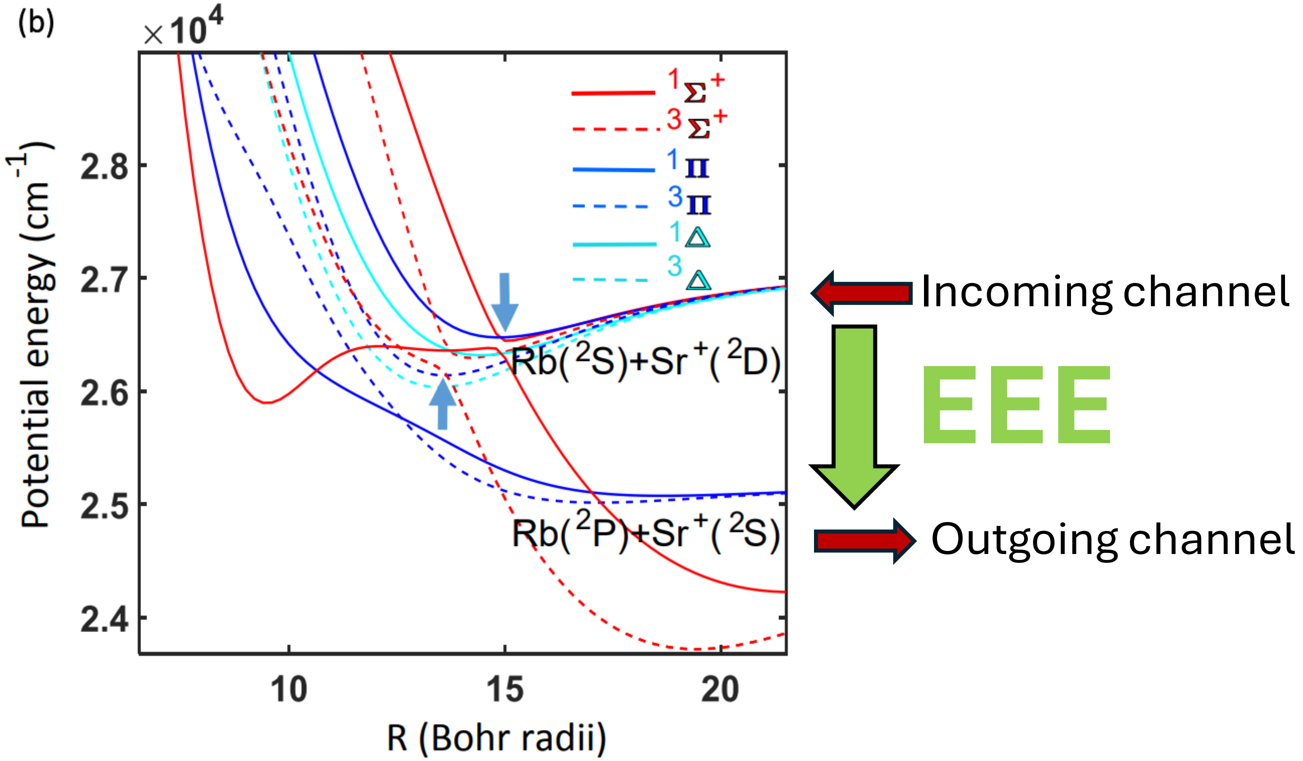

Outlook and perspectives

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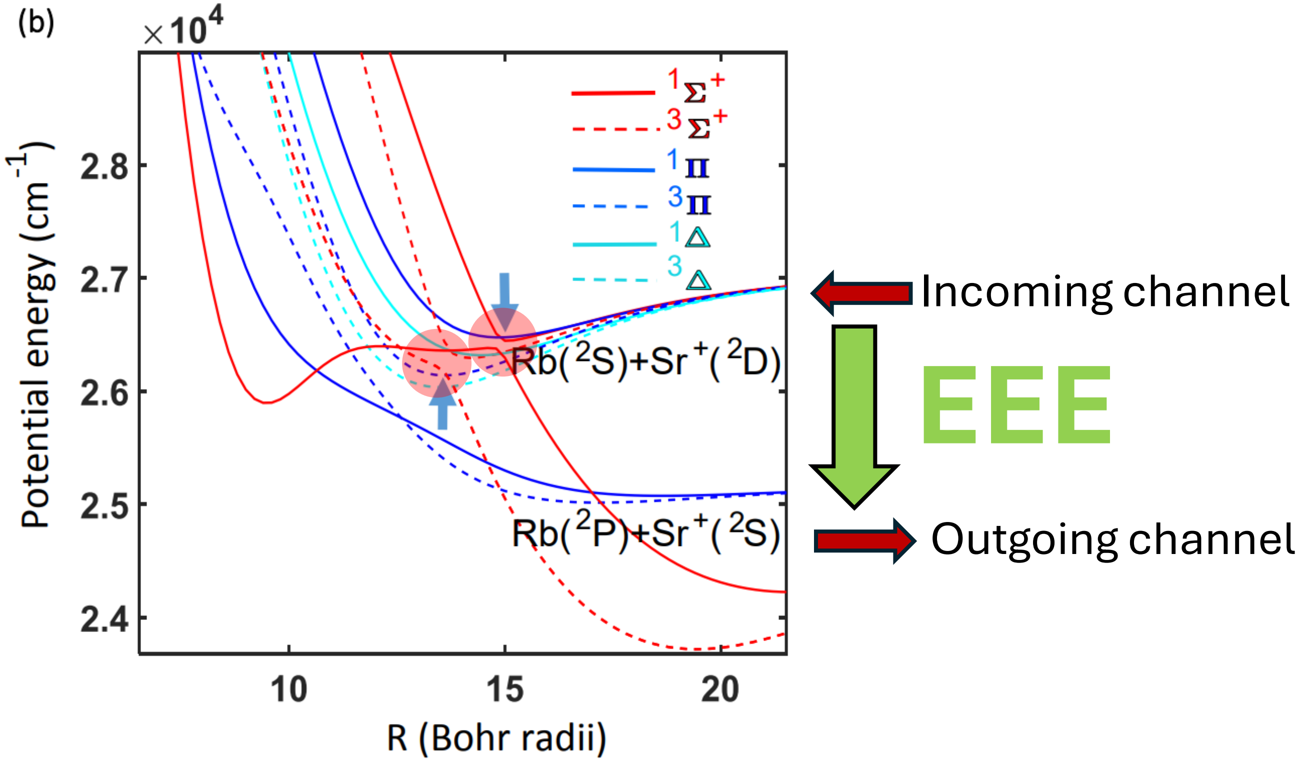
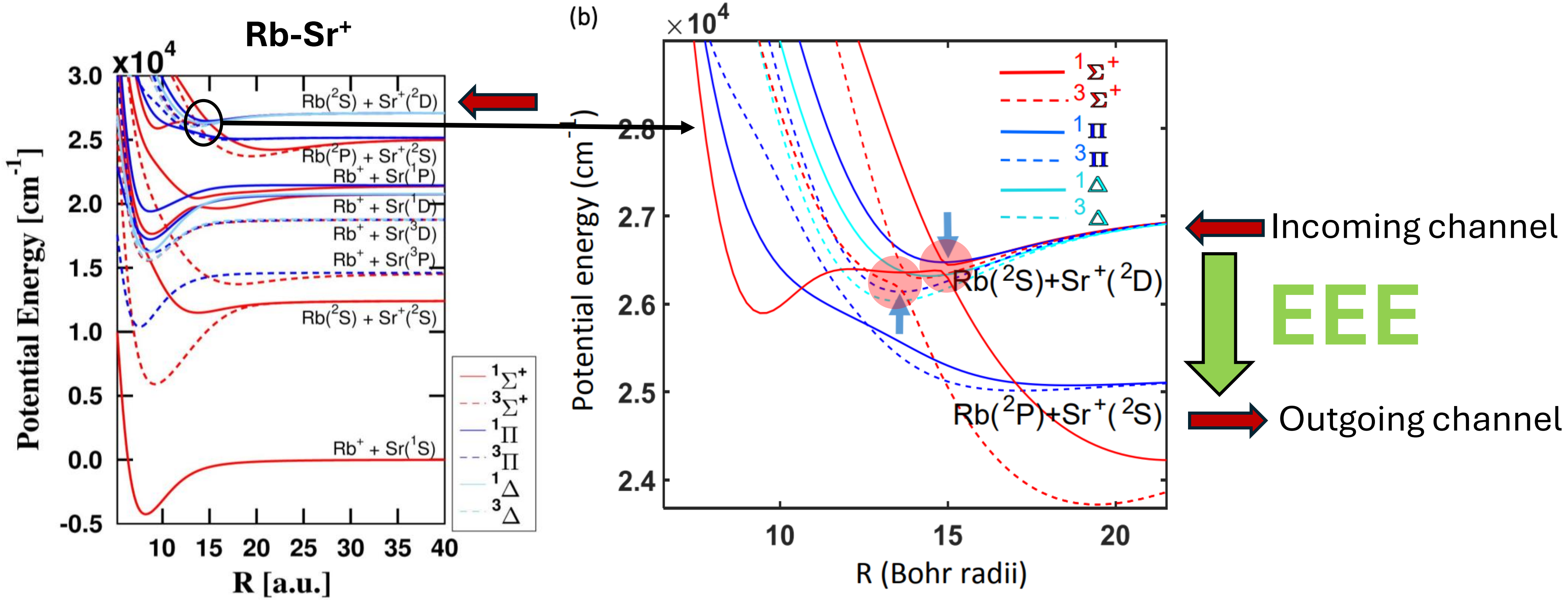


Outlook and perspectives

- Similar investigations for the same class of systems (eg. Rb - Sr^+)
  - different observed process (**electronic excitation exchange, EEE**)
  - more open channel
  - denser asymptotic limits

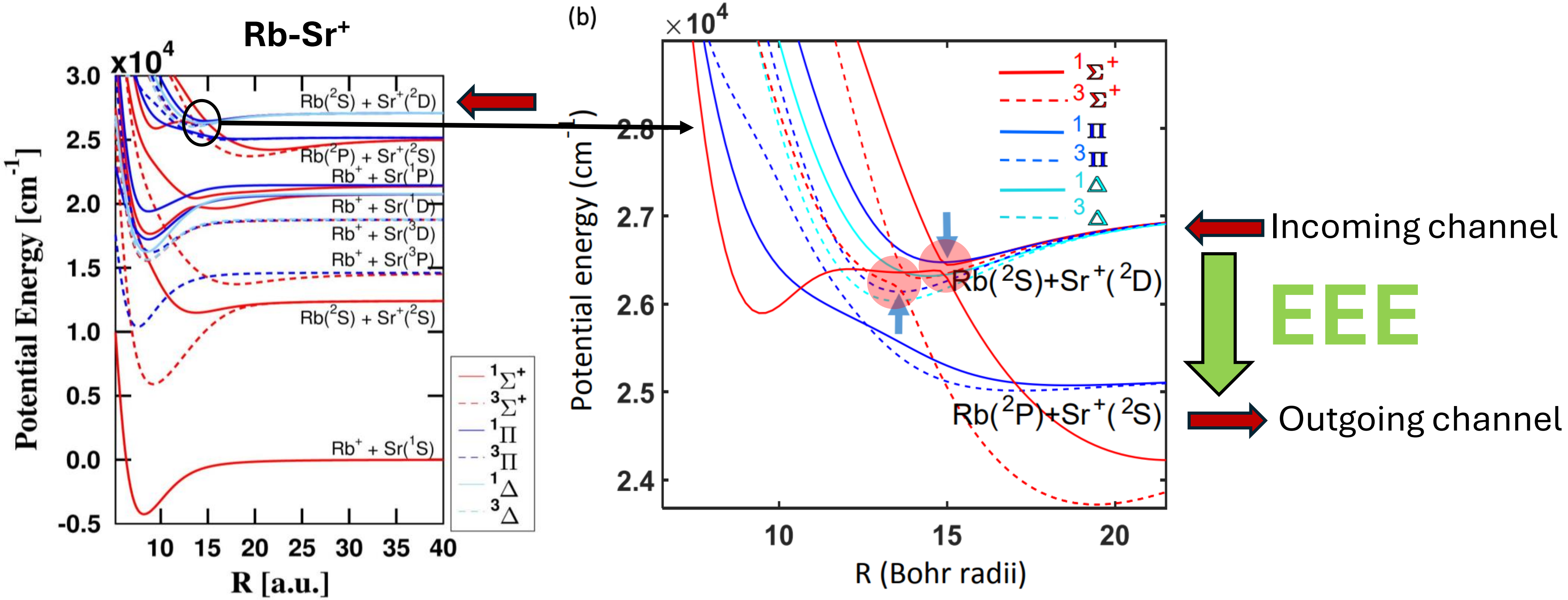
23×23



Outlook and perspectives

- Similar investigations for the same class of systems (eg. Rb - Sr^+)
  - different observed process (**electronic excitation exchange, EEE**)
  - more open channel
  - denser asymptotic limits
- Considering spin – polarization of colliding partners in the model

23×23



Collaboration

- **THEOMOL group, Aimé Cotton Lab., Orsay, France & HUN-REN ATOMKI, Debrecen, Hungary**
  Olivier Dulieu, Nadia Bouloufa-Maafa, Eliane Luc, Romain Vexiau, Xiadong Xing, Ting Xie
  Andrea Orbán
- **Quantum and Atomic Physics group, Uni. Freiburg & Uni. British Columbia, Vancouver, Canada**
  Pascal Weckesser, Fabian Thielemann, Tobias Schaetz
  Kirk W. Madison

Fundings

CNRS International Emerging Action (IEA) – ELKH, 2023-2024

Program Hubert Curien „BALATON" (CampusFrance-GrantNO.49848TC)

NKFIH TÉT-FR, 2023-2024 (2021-1.2.4- TÉT-2022-00069)

French Governmental Scholarship

University of Debrecen

Thank you for your attention!

Rate ratios

Event	Process	Counts	Ratio(%)	$K_{exp.}/K_L^{exp}$	K_{MCQS}/K_L^{th} ; K_{MCQS-L}/K_L^{th}
$5D_{3/2}$: $K_L^{exp} = 4.69 \times 10^{-9}$ cm$^3/s$; $K_L^{th} = 4.81 \times 10^{-9}$ cm$^3/s$					
	EC	177	-	-	-
Hot	NRQ	302	90.6(16)	$0.154(45)_{stat}(27)_{sys}$	0.21;0.18
Loss	NRCE	31	9.4(16)	$0.016(5)_{stat}(3)_{sys}$	0.021;0.012
Total		510			
$5D_{5/2}$: $K_L^{exp} = 4.81 \times 10^{-9}$ cm$^3/s$; $K_L^{th} = 4.81 \times 10^{-9}$ cm$^3/s$					
	EC	41	-	-	-
Cold+Hot	FSQ	42+8	66(6)	$0.198(26)_{stat}(40)_{sys}$	1.06;0.725
Loss	NRCE	25	34(6)	$0.102(14)_{stat}(20)_{sys}$	0.052;0.16
Total		116			

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Frame transformation

coordinate system transformation

Molecular frame → Laboratory frame

Transformation

$$\begin{pmatrix} \Psi_1^{lab} \\ \Psi_2^{lab} \\ \cdot \\ \cdot \\ \cdot \\ \Psi_N^{lab} \end{pmatrix} = \begin{pmatrix} t_{11} & \dots & t_{1N} \\ t_{21} & \dots & t_{2N} \\ \cdot & & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & & \cdot \\ t_{N1} & \dots & t_{NN} \end{pmatrix} \begin{pmatrix} \Psi_1^{mol} & \Psi_2^{mol} & \dots & \Psi_N^{mol} \end{pmatrix}$$

$$t_{ij} = < j_a j_b j l J M | \Lambda S \Sigma J M p > = (-1)^{l-\Omega-J} (2 - \delta_{\Lambda,0}\delta_{\Sigma,0})^{-1/2}$$
$$\times [1 + (-1)^{L_a+L_b+l+p}(1 - \delta_{\Lambda,0}\delta_{\Sigma,0})]$$
$$\times \sqrt{(2S+1)(2j_a+1)(2j_b+1)}$$
$$\times < l0 | j - \Omega, J\Omega >< L\Lambda | L_a\Lambda_a, L_b\Lambda_b >$$
$$\times \begin{Bmatrix} L_a & S_a & j_a \\ L_b & S_b & j_b \\ L & S & j \end{Bmatrix} < j\Omega | L\Lambda, S\Sigma >$$

where, $j_{a/b}$ – A/B atom el. angular momentum quantum number

- j – total el. angular momentum quantum number
- l – partial wave quantum number
- J – total angular momentum quantum number
- M – projectile of total angular momentum quantum number
- Λ – projectile of orbital momentum quantum number
- S – spin
- Σ – projectile of spin
- p – parity
- Ω – Λ + Σ
- $< \cdots | \cdots >$ – Clebsch – Gordan coeffcient
- $\{ \cdots \}$ – 9-j symbol