Few-body processes in cold chemistry

Jesús Pérez-Ríos

FRITZ-HABER-INSTITUT
MAX-PLANCK-GESELLSCHAFT

https://fhi.iwww.mpg.de/209391/AMO_theory

The team

FRITZ-HABER-INSTITUT
MAX-PLANCK-GESELLSCHAFT

Xiangyue Liu

Marjan Mirahmadi

Miruna Cretu

https://fhi.iwww.mpg.de/209391/AMO_theory

Introduction

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Few-body physics

Cold chemistry

Impurity physics

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Few-body physics

Cold chemistry

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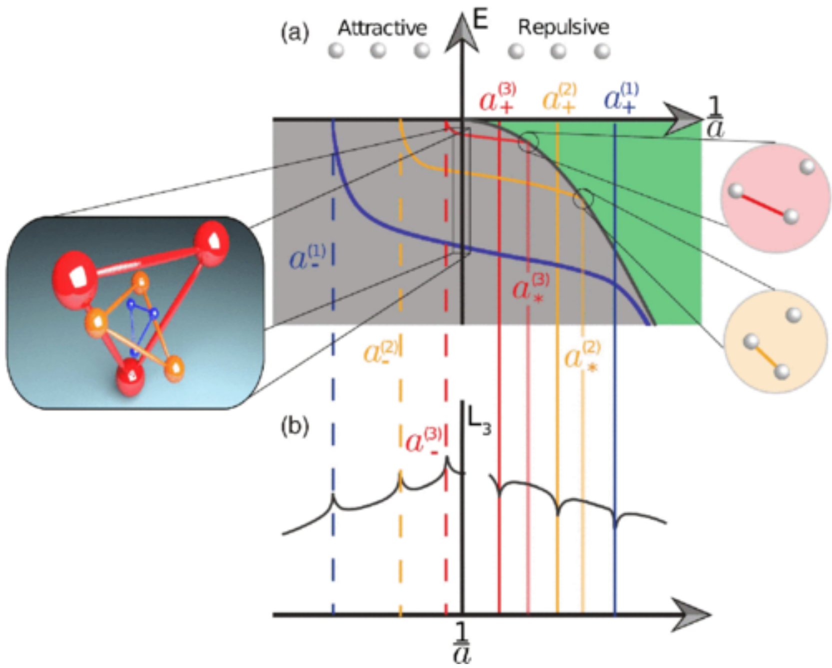
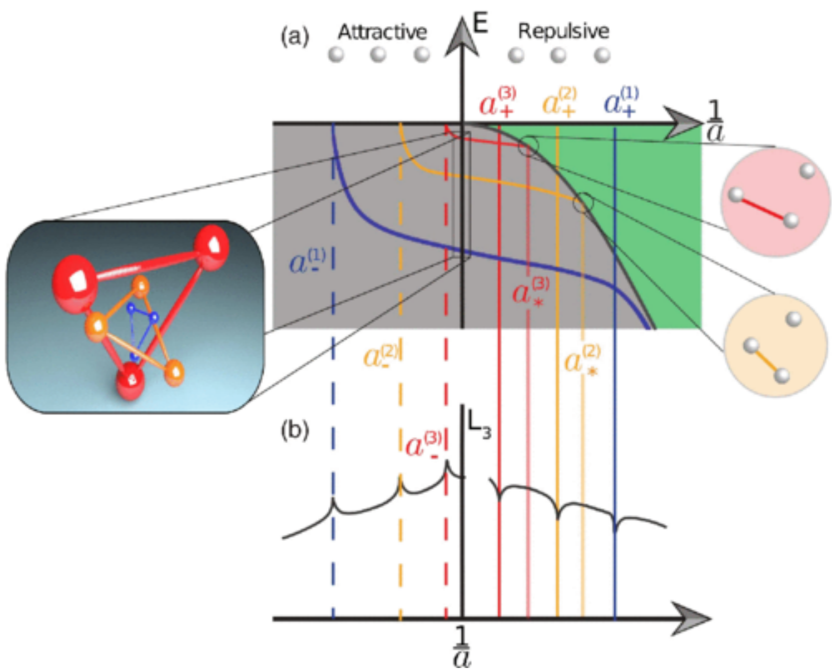


REVIEWS OF MODERN PHYSICS, VOLUME 89, JULY–SEPTEMBER 2017

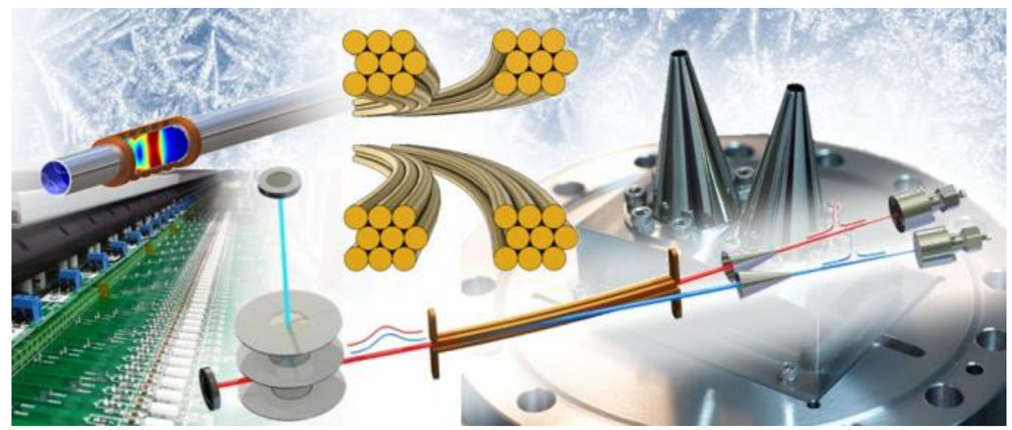
Universal few-body physics and cluster formation

Chris H. Greene,[*] P. Giannakeas,[†] and J. Pérez-Ríos[‡]

Few-body physics



Cold chemistry



Observation of Resonances in Penning Ionization Reactions at Sub-Kelvin Temperatures in Merged Beams

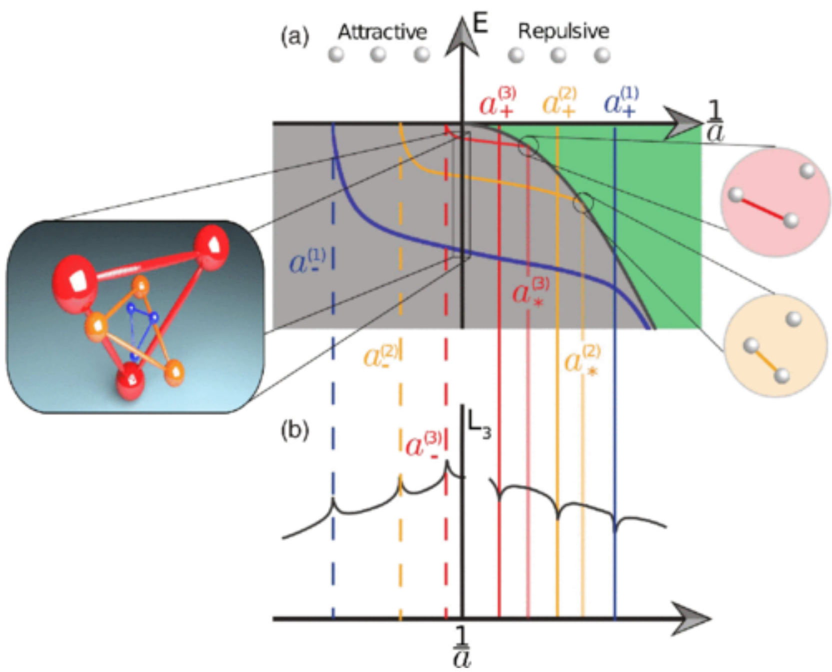
A. B. Henson, S. Gersten, Y. Shagam, J. Narevicius, E. Narevicius*

12 OCTOBER 2012 VOL 338 **SCIENCE** www.sciencemag.org

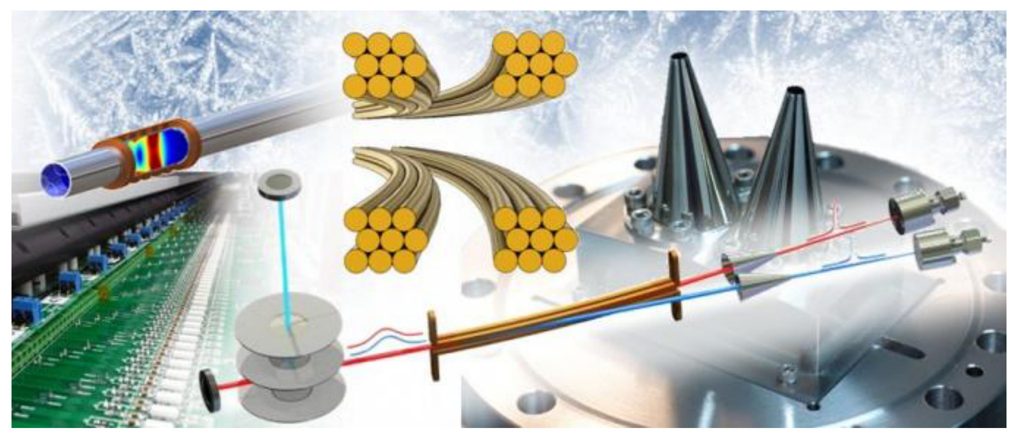
Impurity physics

Introduction

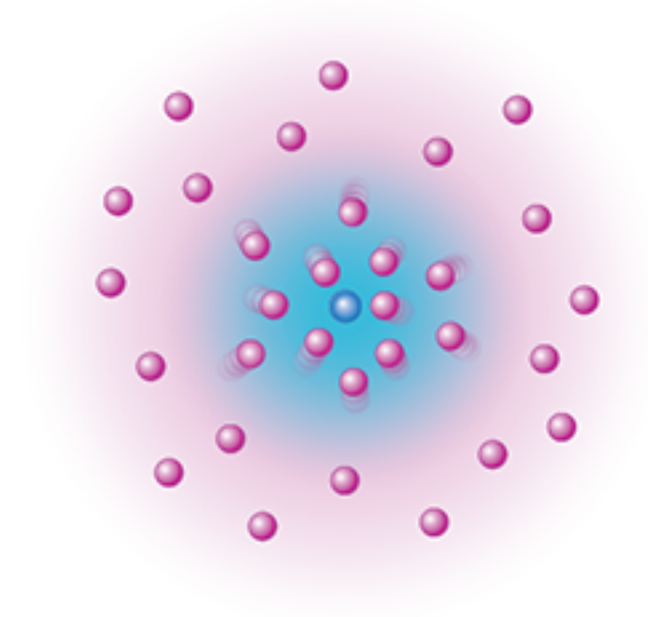
Few-body physics



Cold chemistry



Impurity physics



Selected for a Viewpoint in *Physics*
PRL **117,** 055302 (2016) PHYSICAL REVIEW LETTERS week ending 29 JULY 2016

Observation of Attractive and Repulsive Polarons in a Bose-Einstein Condensate

Nils B. Jørgensen,[1] Lars Wacker,[1] Kristoffer T. Skalmstang,[1] Meera M. Parish,[2] Jesper Levinsen,[2]
Rasmus S. Christensen,[1] Georg M. Bruun,[1] and Jan J. Arlt[1]

Selected for a Viewpoint in *Physics*
PRL **117,** 055301 (2016) PHYSICAL REVIEW LETTERS week ending 29 JULY 2016

Bose Polarons in the Strongly Interacting Regime

Ming-Guang Hu, Michael J. Van de Graaff, Dhruv Kedar, John P. Corson, Eric A. Cornell, and Deborah S. Jin

Introduction

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Few-body physics: deals with systems with few degrees of freedom

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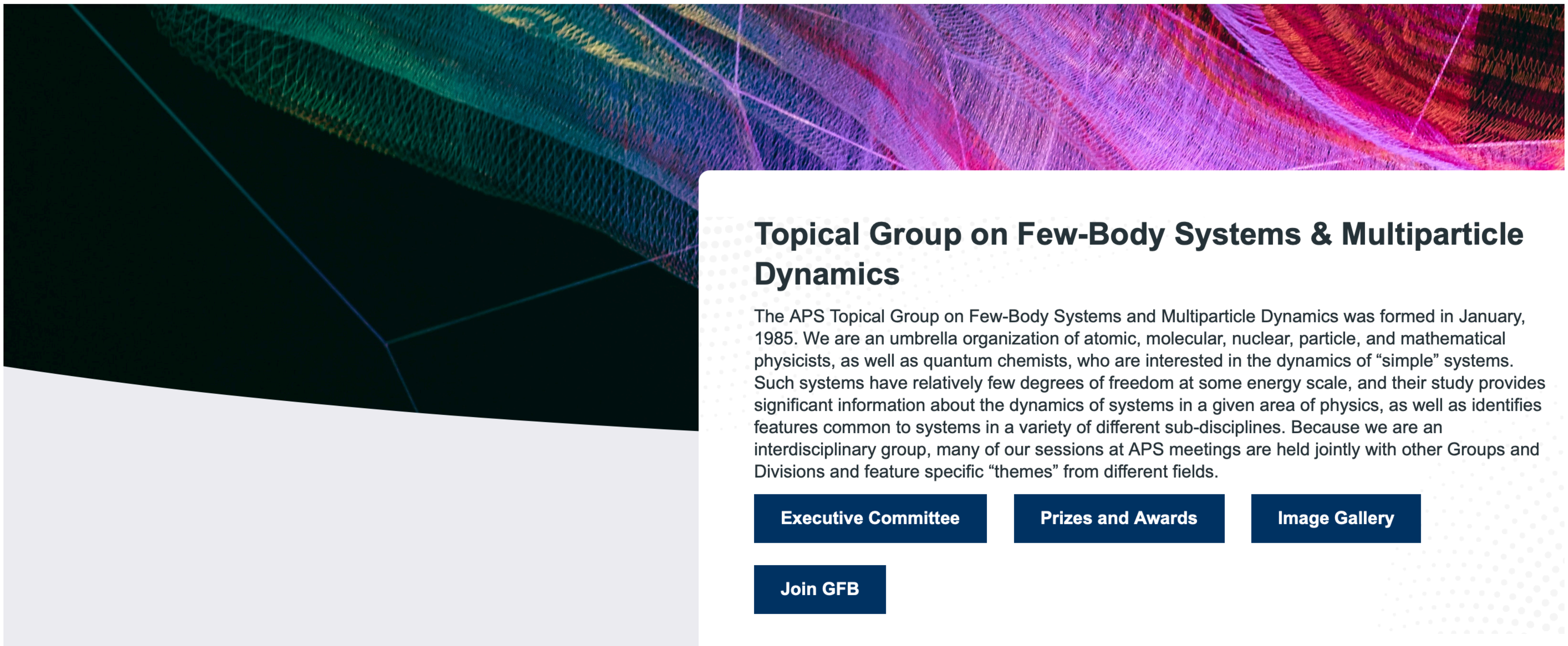
Few-body physics: deals with systems with few degrees of freedom

APS physics — **Topical Group on Few-Body Systems & Multiparticle Dynamics**



Topical Group on Few-Body Systems & Multiparticle Dynamics

The APS Topical Group on Few-Body Systems and Multiparticle Dynamics was formed in January, 1985. We are an umbrella organization of atomic, molecular, nuclear, particle, and mathematical physicists, as well as quantum chemists, who are interested in the dynamics of “simple” systems. Such systems have relatively few degrees of freedom at some energy scale, and their study provides significant information about the dynamics of systems in a given area of physics, as well as identifies features common to systems in a variety of different sub-disciplines. Because we are an interdisciplinary group, many of our sessions at APS meetings are held jointly with other Groups and Divisions and feature specific “themes” from different fields.

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Few-body physics: deals with systems with few degrees of freedom

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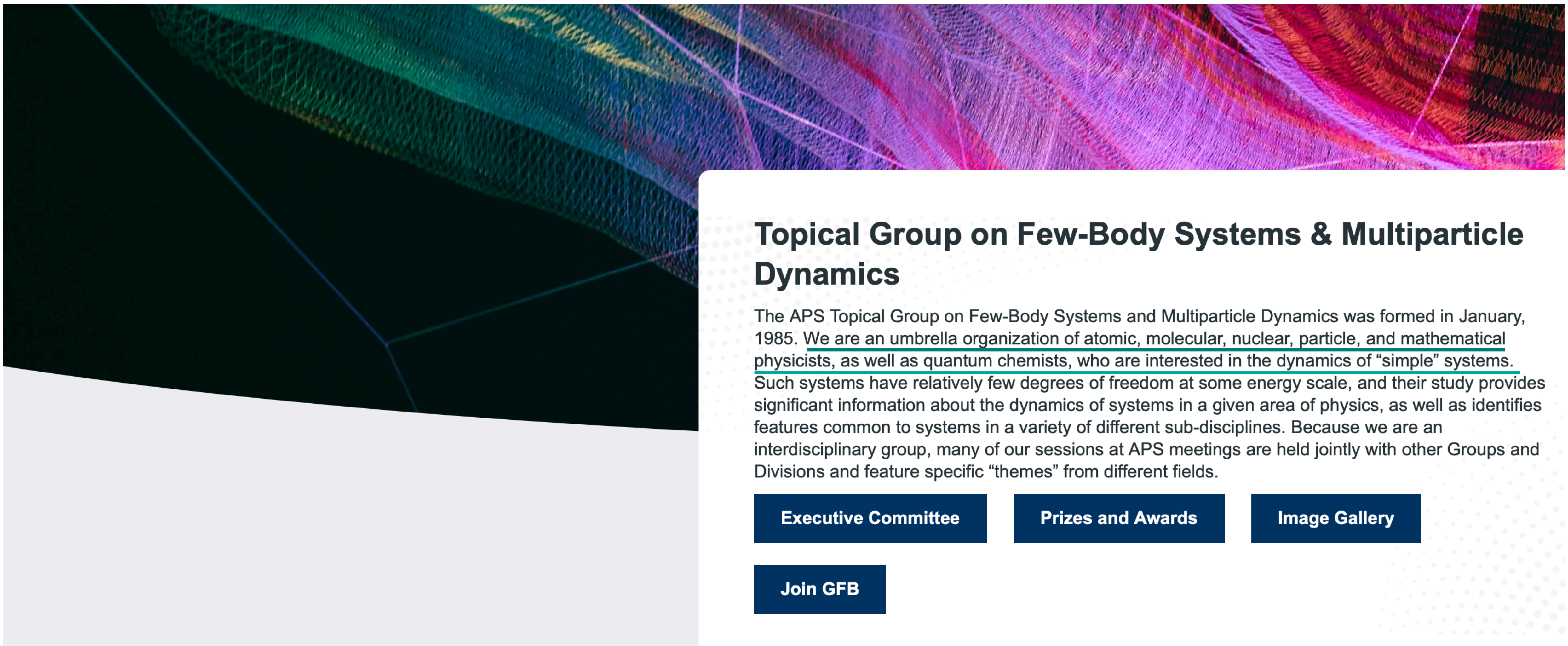

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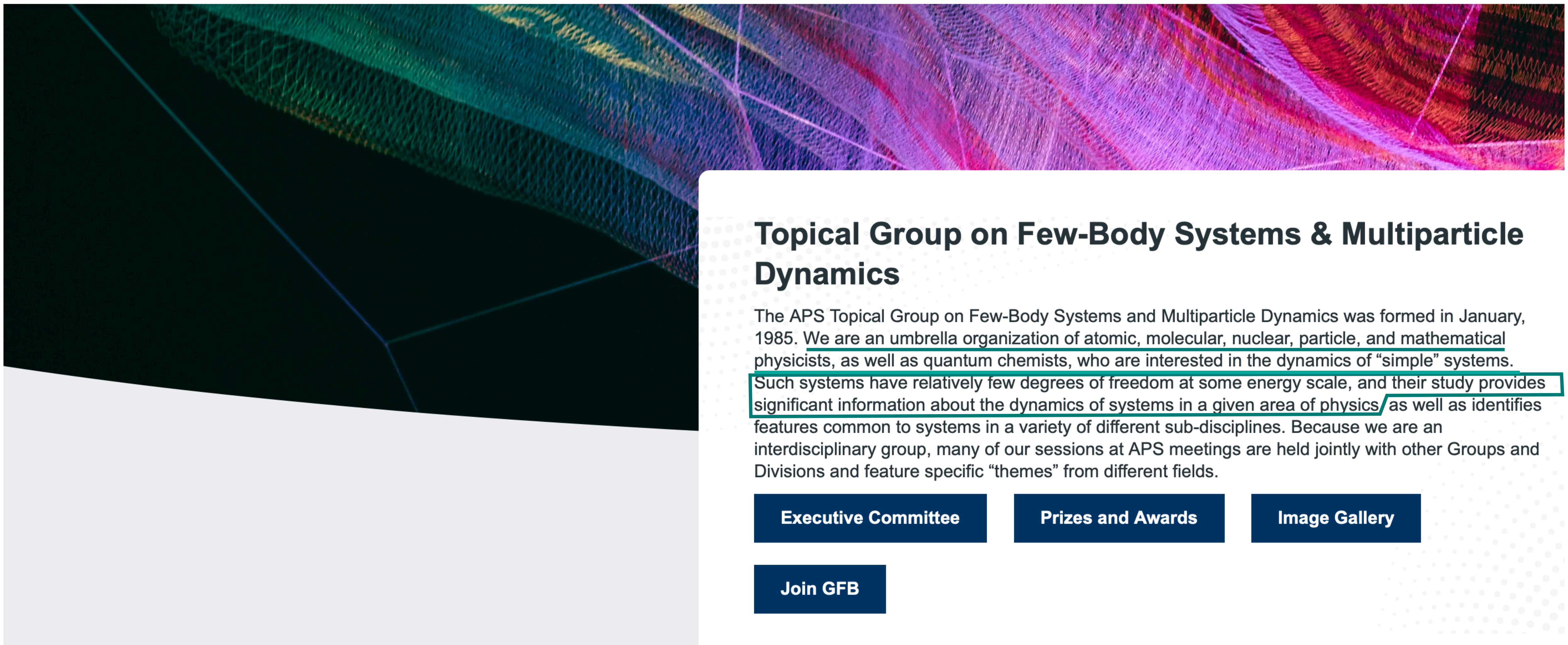

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Chris H. Greene,[*] P. Giannakeas,[†] and J. Pérez-Ríos[‡]

Chemical reactions are few-body processes

Introduction

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Cold chemistry: **study of chemical reactions below 1K up to 1 mK**

Introduction

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Cold chemistry: study of chemical reactions below 1K up to 1 mK

PERSPECTIVE www.rsc.org/pccp | Physical Chemistry Chemical Physics

Cold controlled chemistry

R. V. Krems

Received 11th February 2008, Accepted 9th April 2008
First published as an Advance Article on the web 20th May 2008
DOI: 10.1039/b802322k

- Quantum effects
- Tunability through external fields

Introduction

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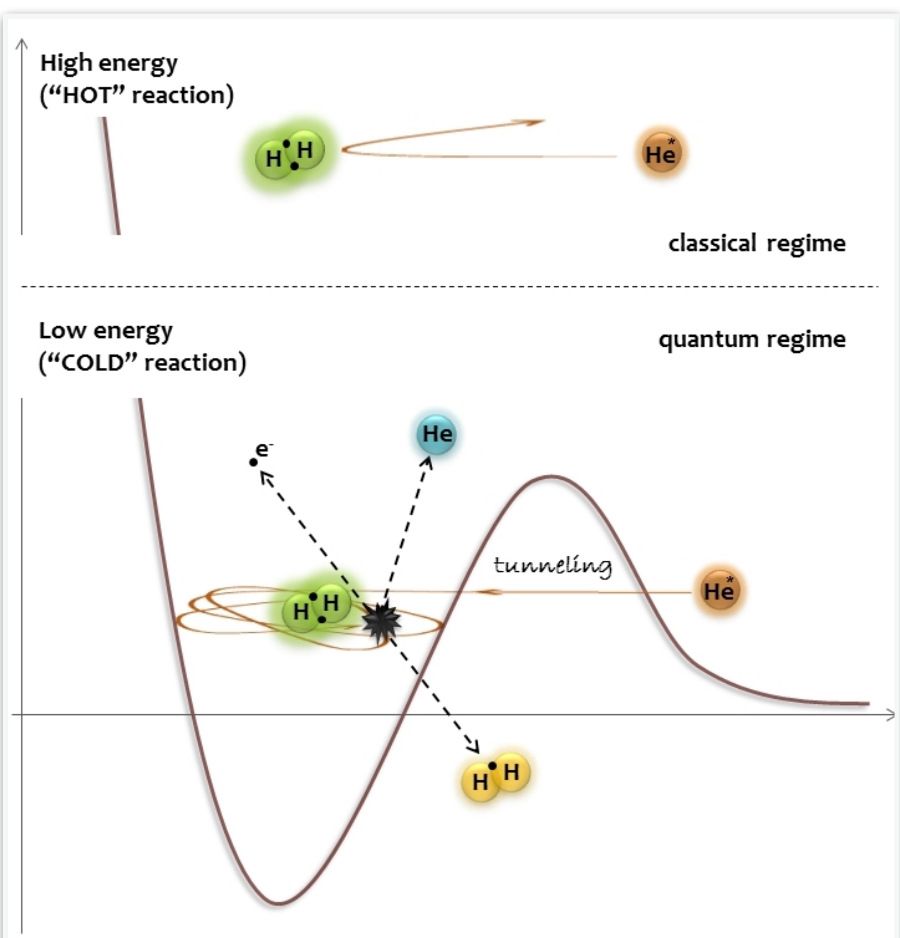

Narevicius' group at the Weizmann Institute of Science

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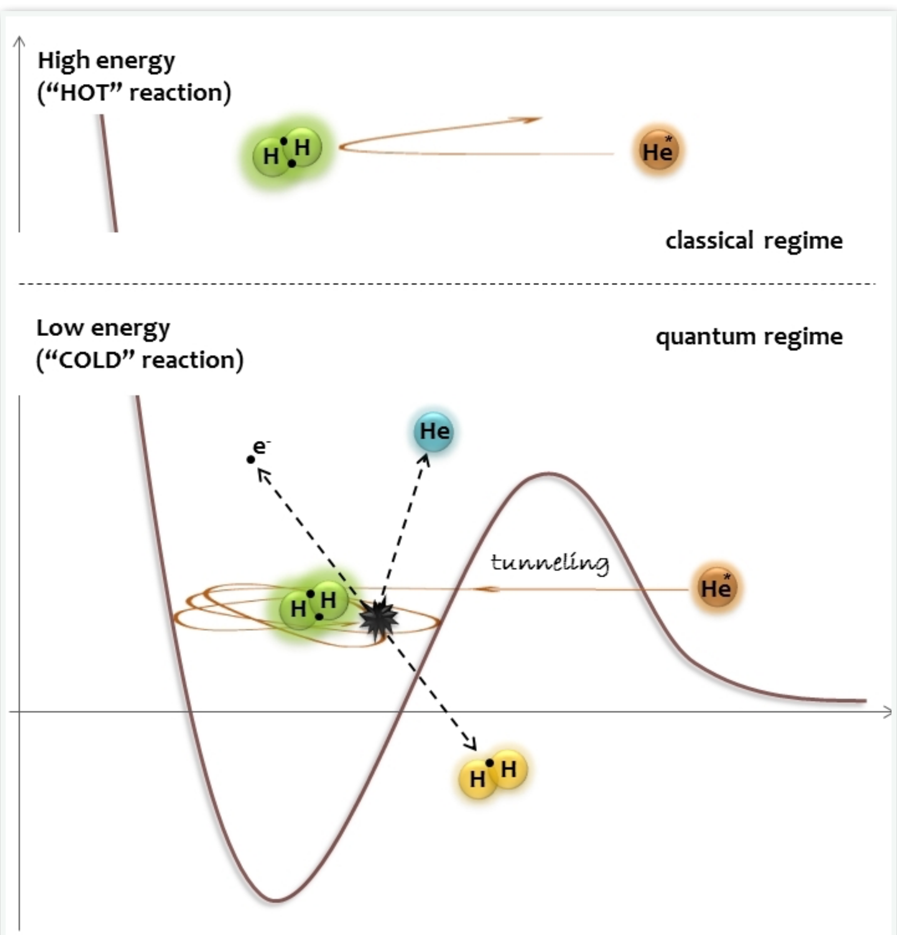

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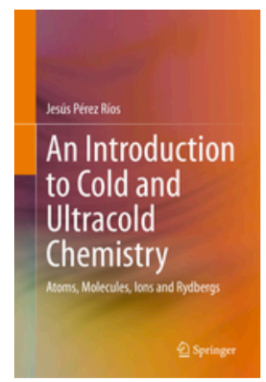

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An Introduction to Cold and Ultracold Chemistry

Atoms, Molecules, Ions and Rydbergs

Authors: **Pérez Ríos**, Jesús

Provides readers with an overview of the fundamentals in cold and ultracold chemistry

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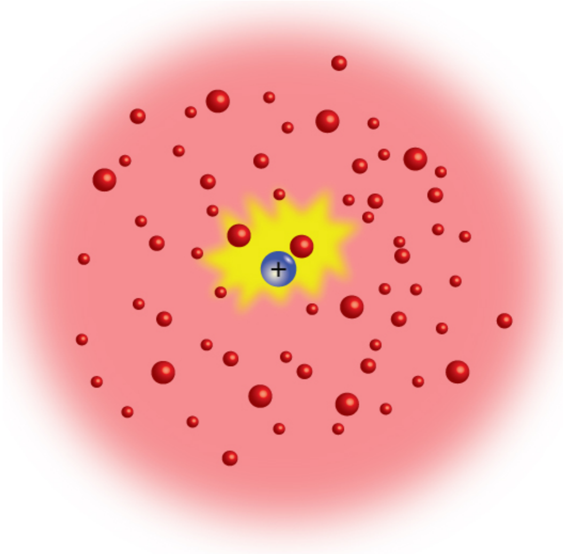
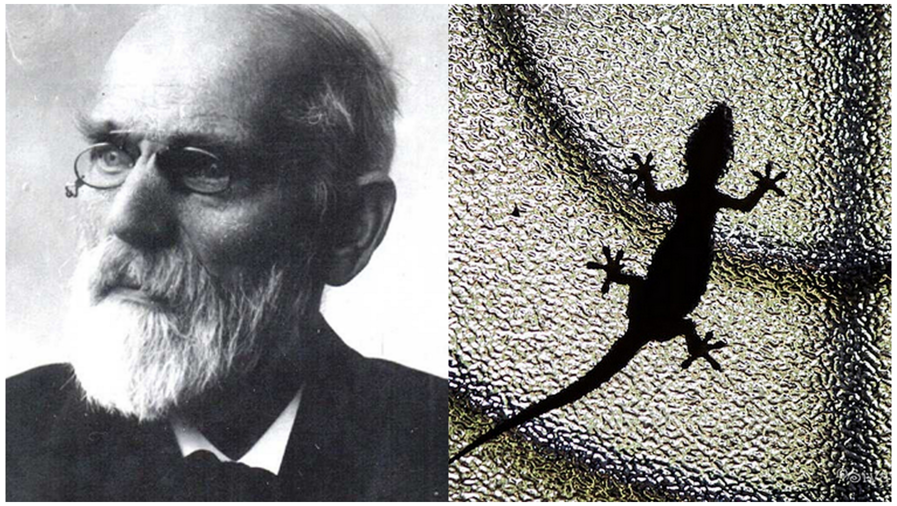
Narevicius' group at the Weizmann Institute of Science

Outlook

A single ion in an ultracold bath



Formation of van der Waals molecules



Outlook

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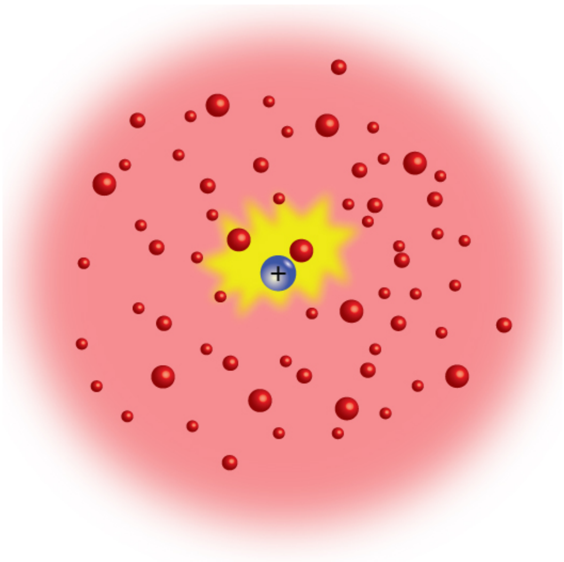
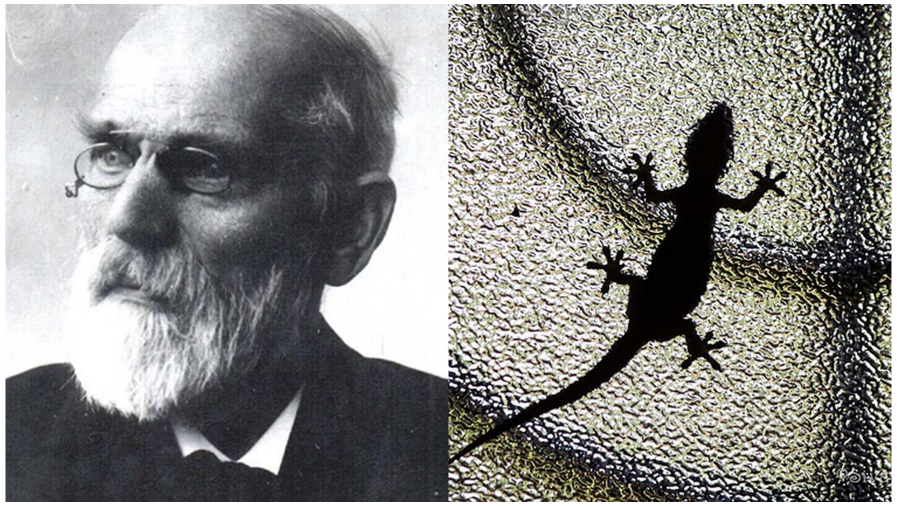


Formation of van der Waals molecules



Outlook

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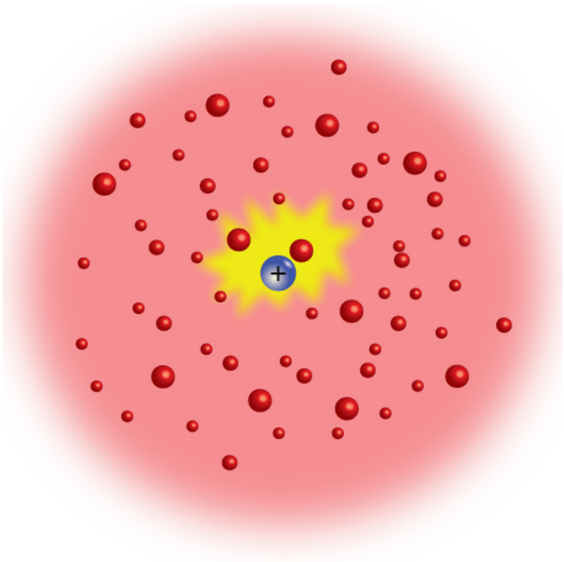
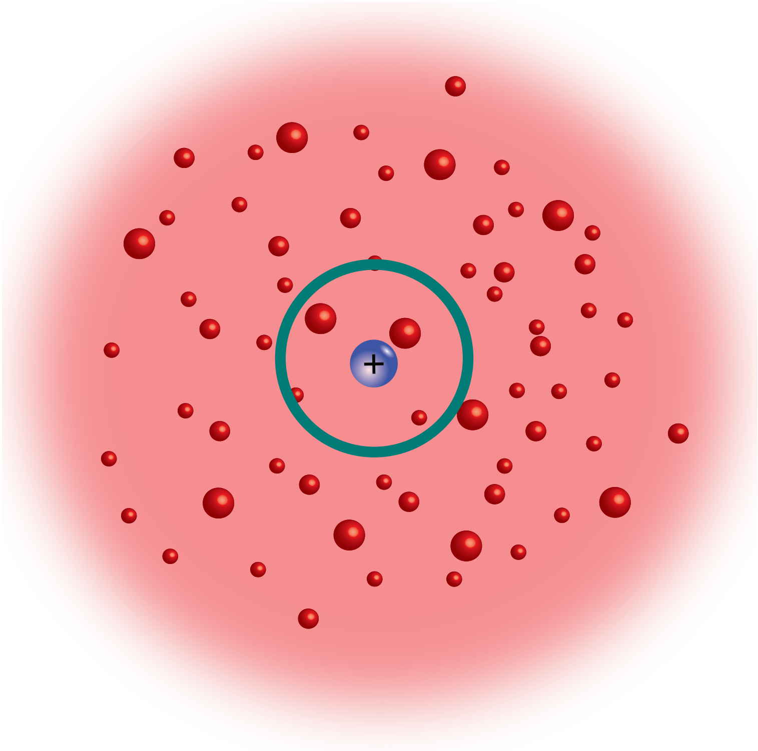


Formation of van der Waals molecules

A single ion in a bath of ultracold atoms

Ion-atom-atom three-body recombination



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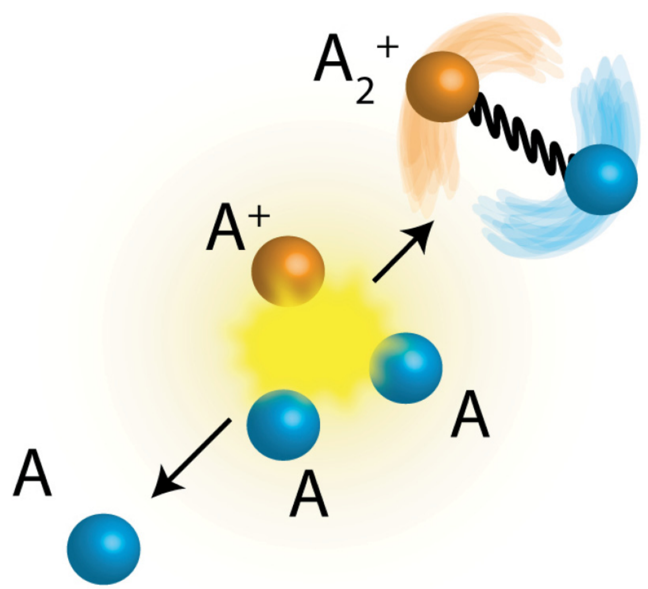
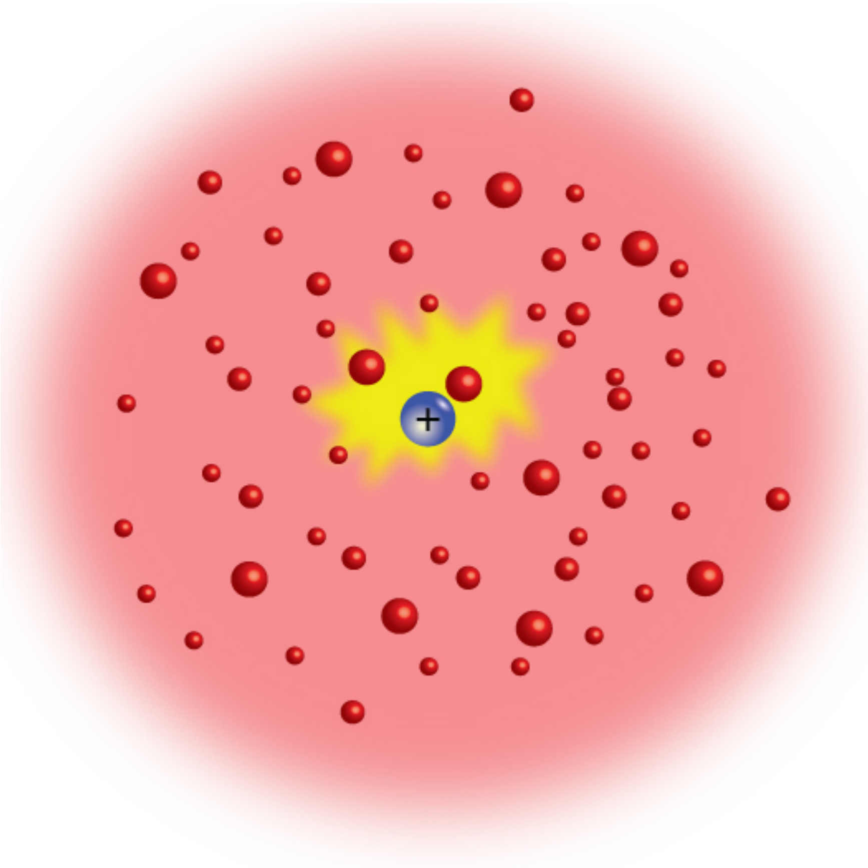
Ion-atom-atom three-body recombination

Three-body recombination

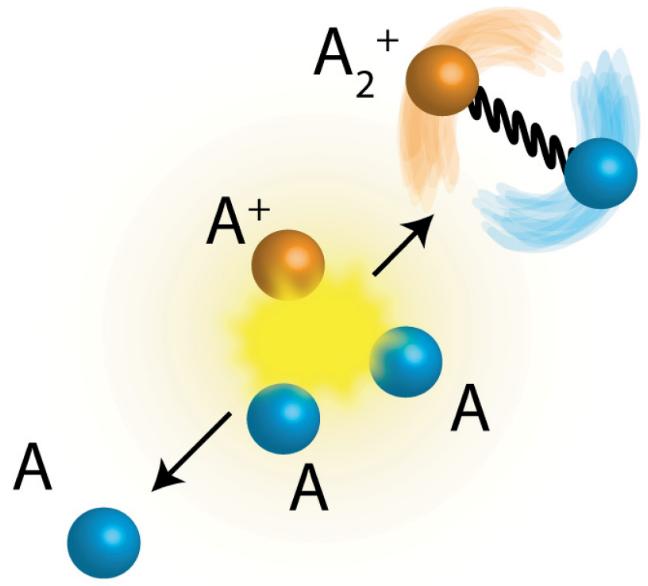




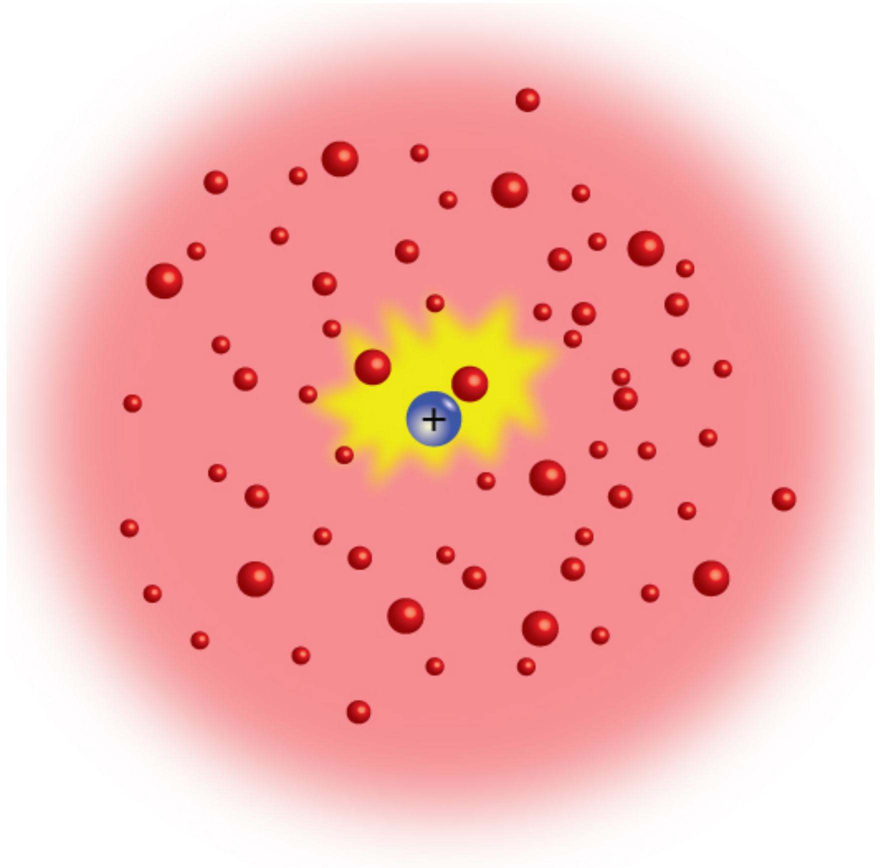
A single ion in a bath of ultracold atoms

Ion-atom-atom three-body recombination

Three-body recombination



$$A^+ + A + A \rightarrow A_2^+ + A$$
$$\rightarrow A_2 + A^+$$



Ion-atom-atom three-body recombination

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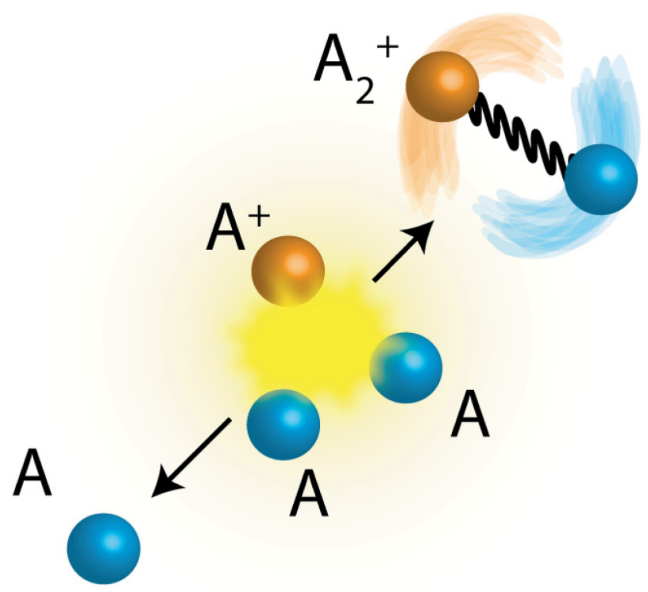
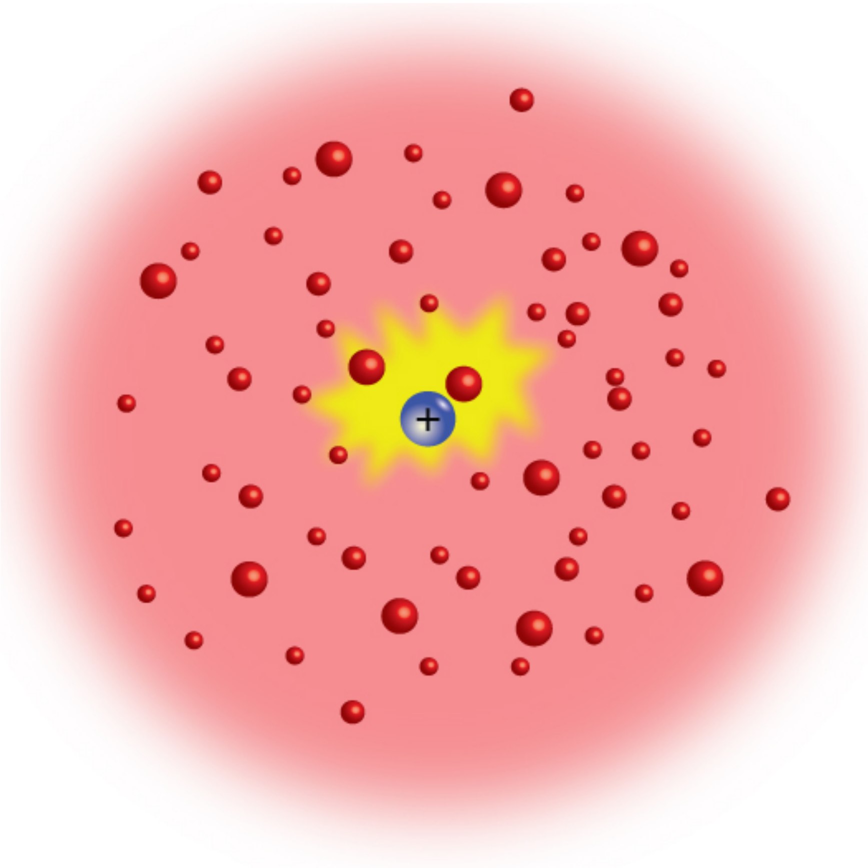




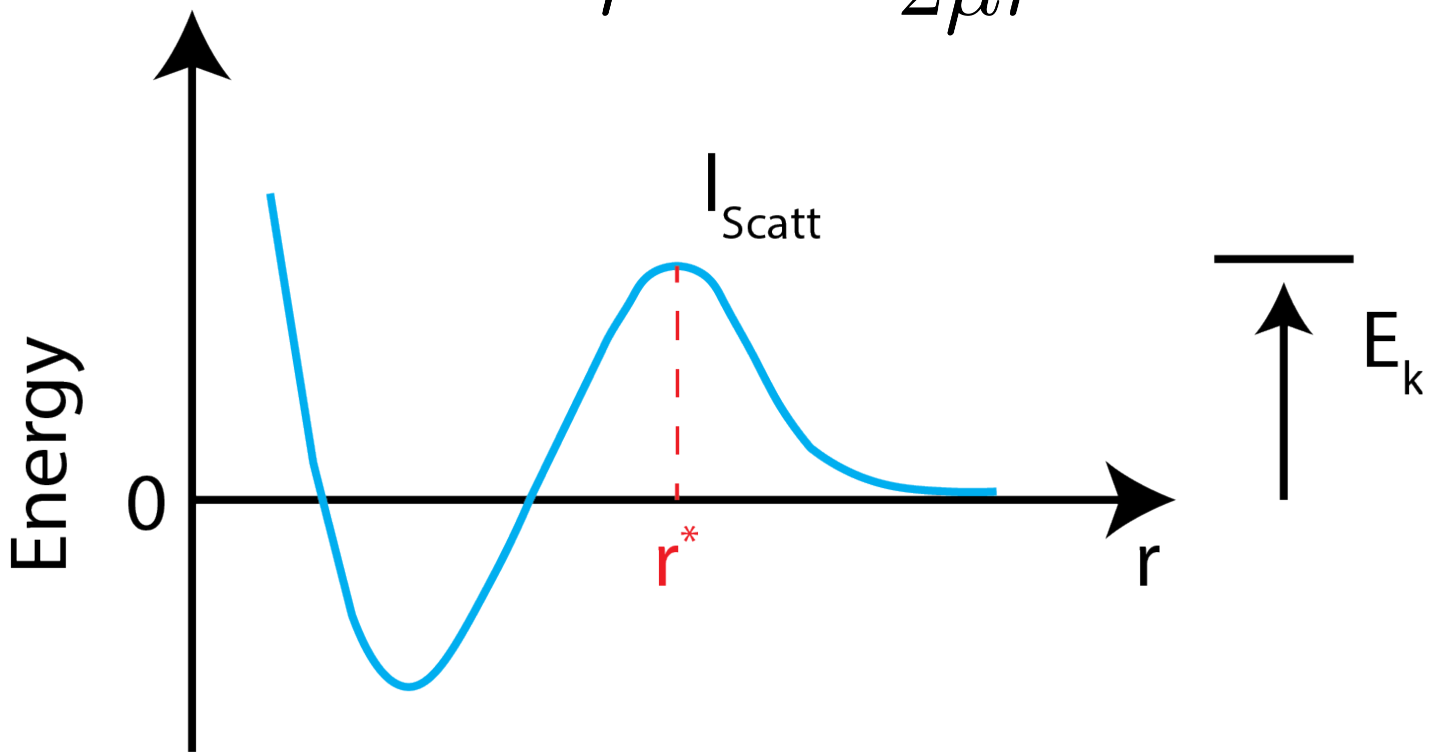
$$A^+ + A + A \rightarrow A_2^+ + A$$
$$\rightarrow A_2 + A^+$$

Only efficient at high densities

Ion-atom-atom three-body recombination

Validity of a classical treatment

$$V_{\mathrm{eff}}(r) = -\frac{C_n}{r^n} + \frac{l(l+1)}{2\mu r^2}$$



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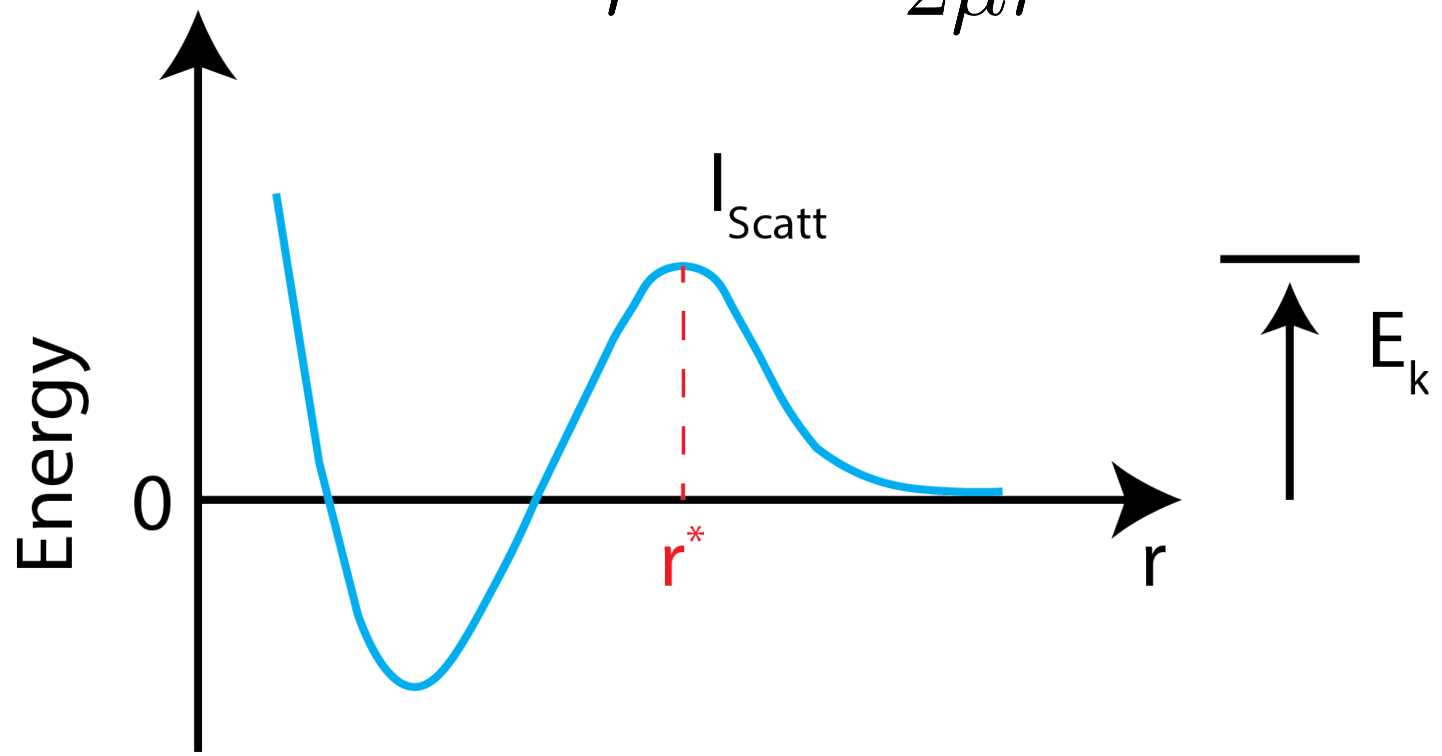
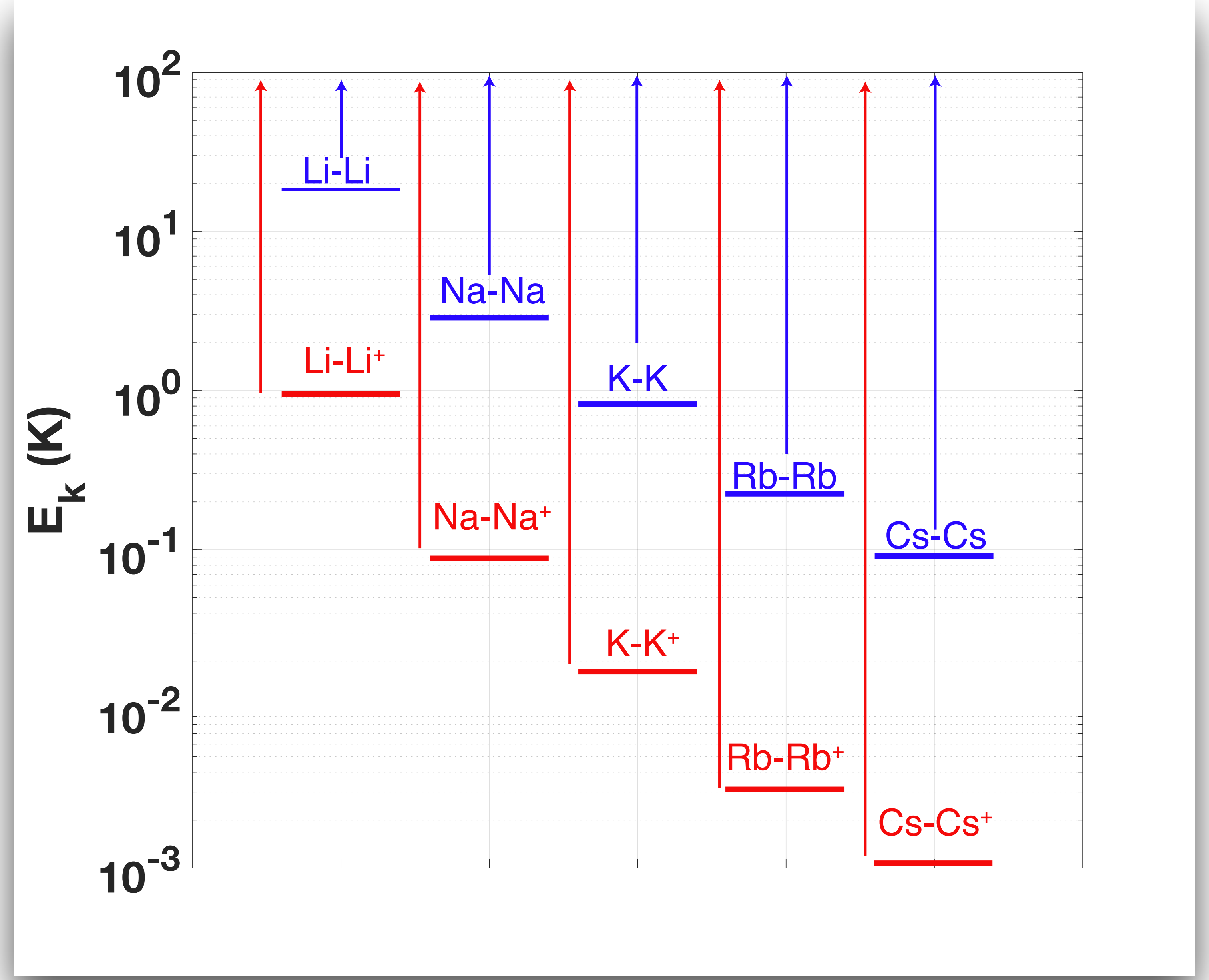


$$l_{\rm Scatt} = \left(\frac{2}{n-2}\right)^{\frac{n-2}{2n}} \sqrt{n\mu C_n^{1/n} E_k^{\frac{n-2}{2n}}}$$

A single ion in a bath of ultracold atoms

Ion-atom-atom three-body recombination

Validity of a classical treatment



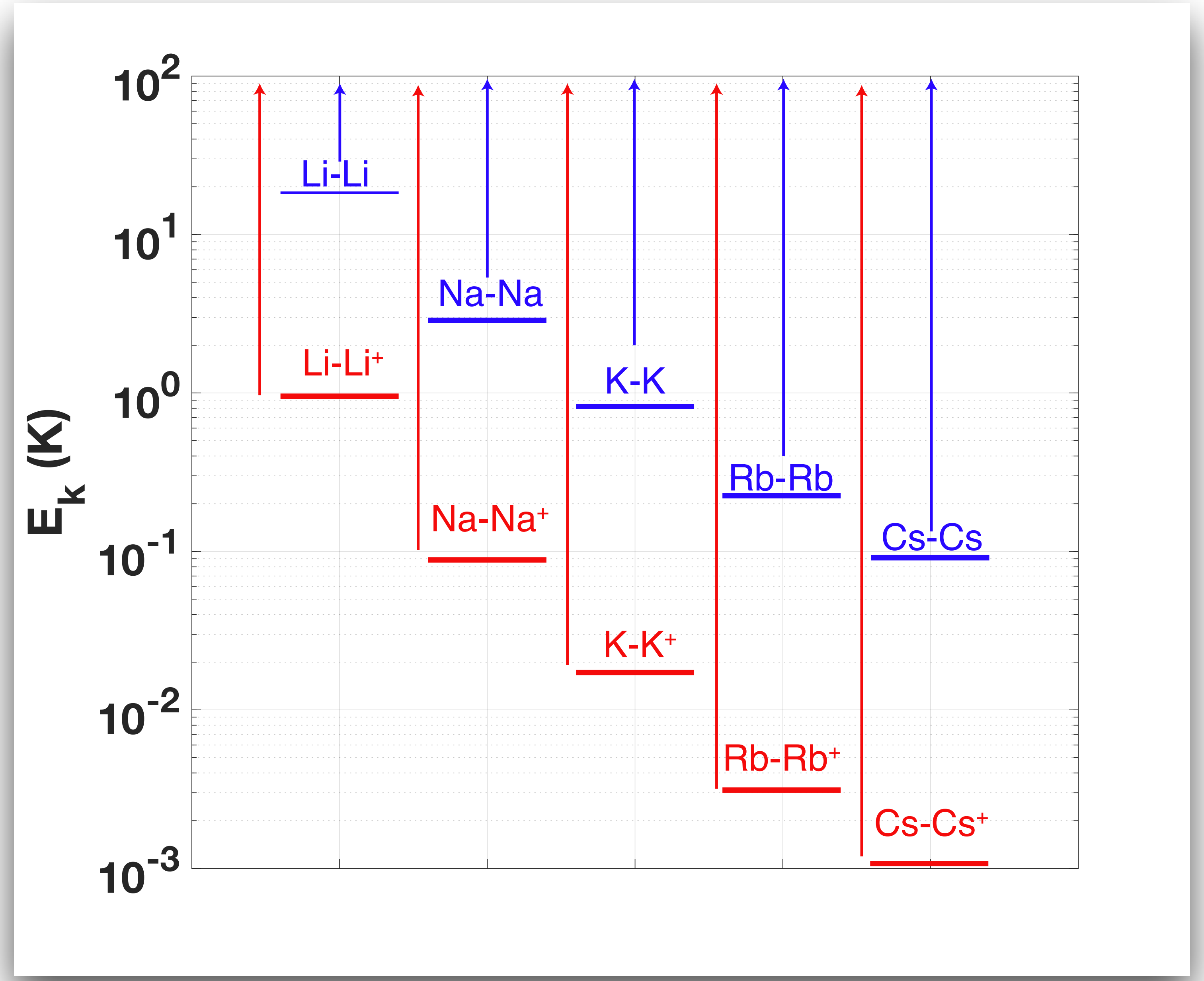
$$l_{\rm Scatt} \sim 20$$

J. Pérez-Ríos, PRA **99**, 022707 (2019)

A single ion in a bath of ultracold atoms

Ion-atom-atom three-body recombination

Validity of a classical treatment



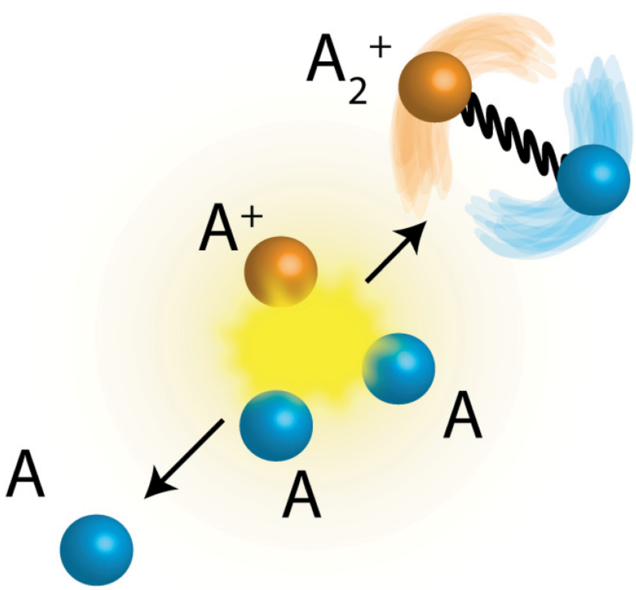
$$l_{\mathrm{Scatt}} \sim 20$$

Cold collision between charged and neutral particles can be treated classically

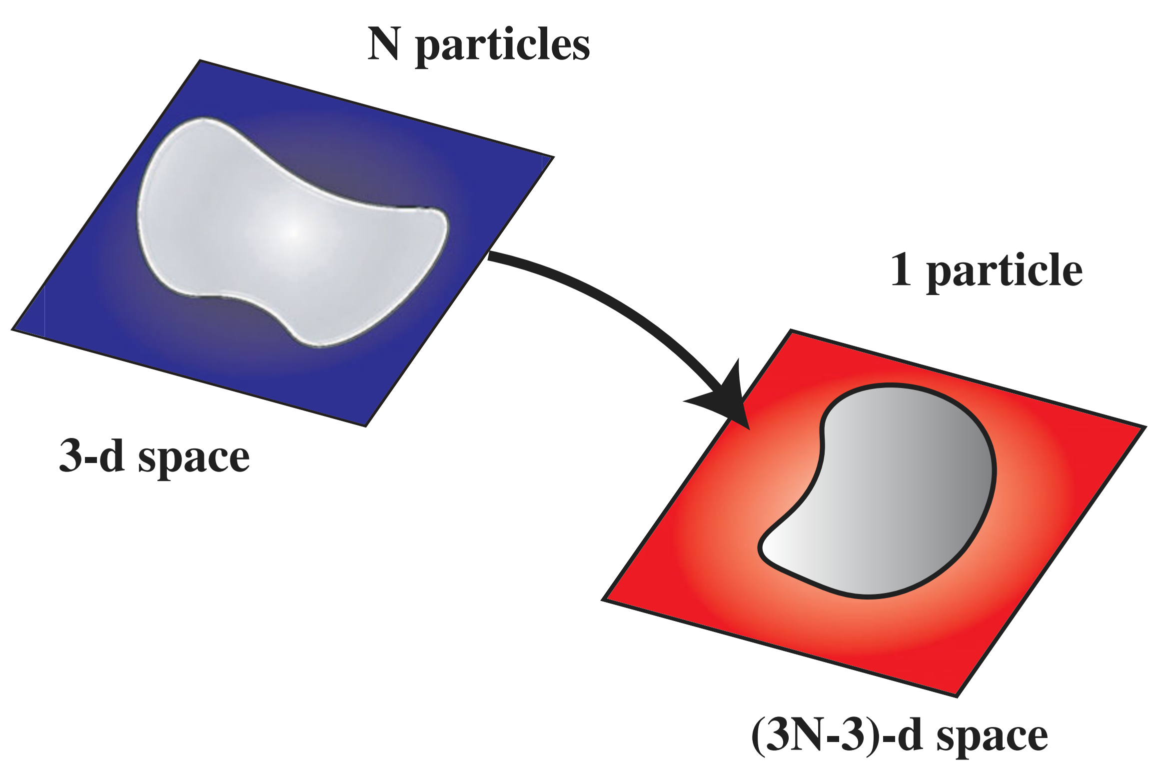
J. Pérez-Ríos, PRA **99**, 022707 (2019)

A single ion in a bath of ultracold atoms

Ion-atom-atom three-body recombination



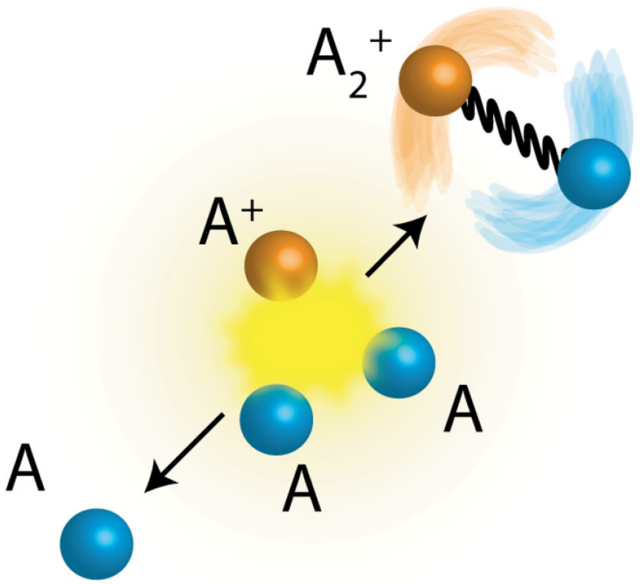
Classical trajectory calculations



C. H. Greene et al., Rev. Mod. Phys. **89**, 035006 (2017)

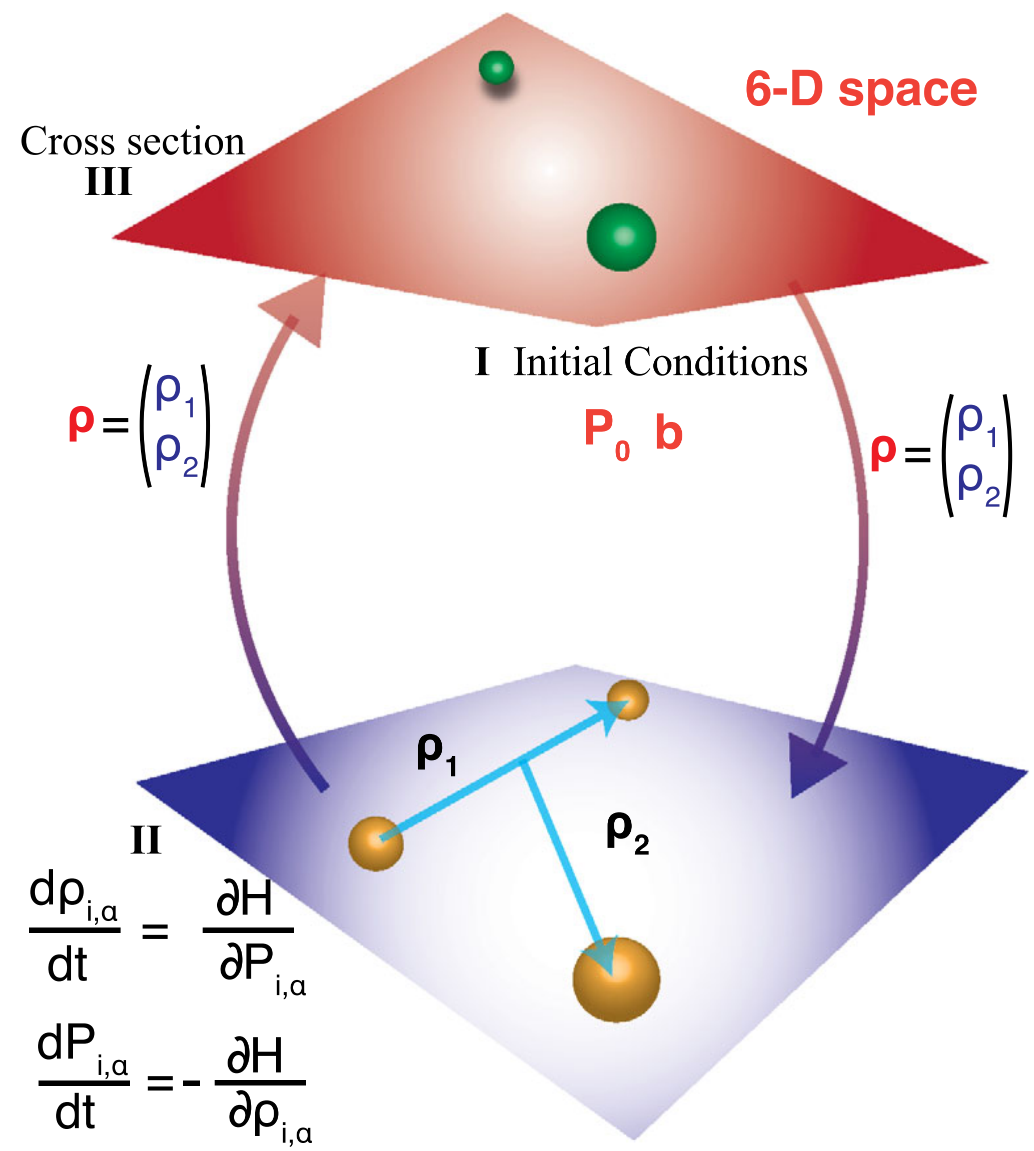
A single ion in a bath of ultracold atoms

Ion-atom-atom three-body recombination



$$H = \frac{\boldsymbol{P}_1^2}{2m_{12}} + \frac{\boldsymbol{P}_2^2}{2m_{3,12}} + V(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2).$$

Classical trajectory calculations



C. H. Greene et al., Rev. Mod. Phys. **89**, 035006 (2017)

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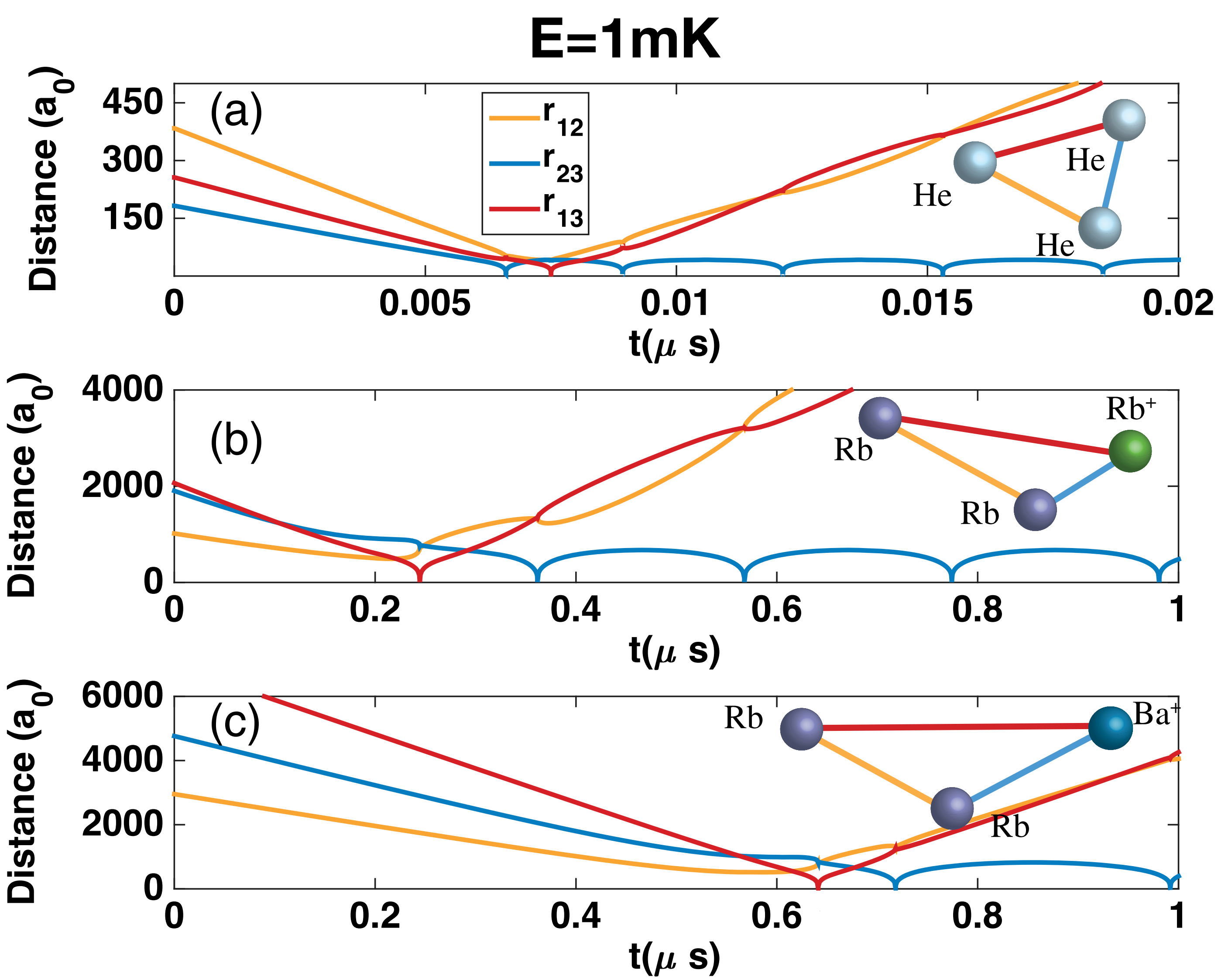


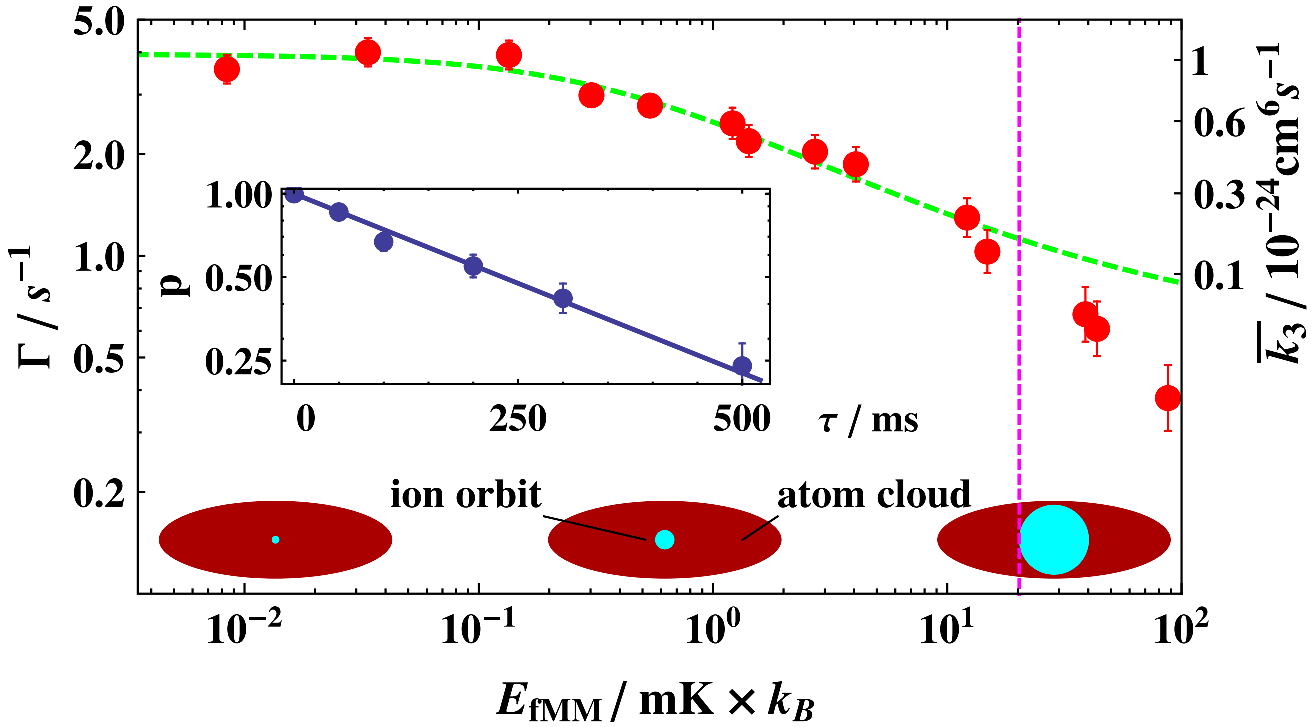
C. H. Greene et al., Rev. Mod. Phys. **89**, 035006 (2017)

A single ion in a bath of ultracold atoms

Ion-atom-atom three-body recombination

Ba+ + Rb +Rb

Classical trajectory calculations versus experimental results



A. Krükow et al., PRL **116**, 193201 (2016)

A single ion in a bath of ultracold atoms

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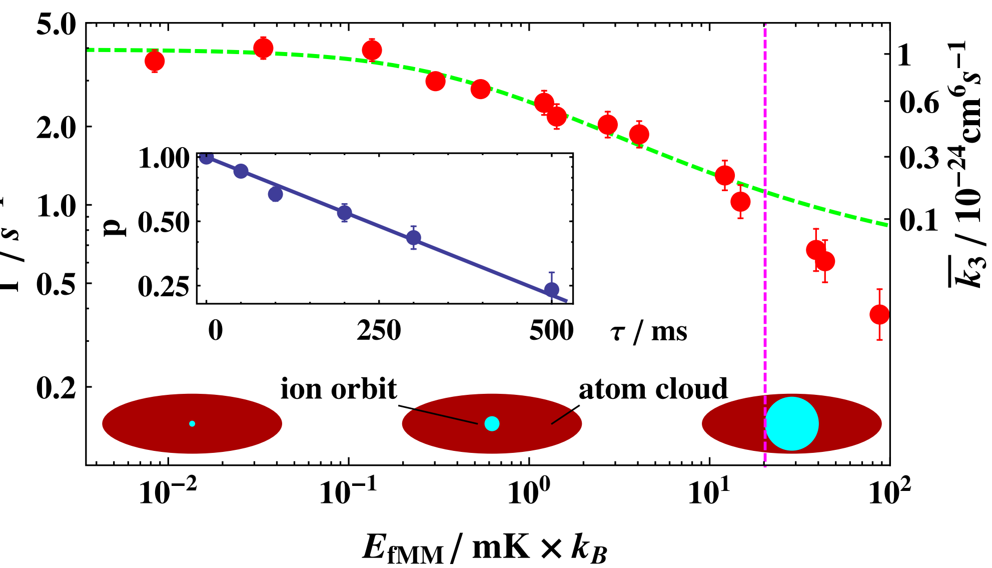
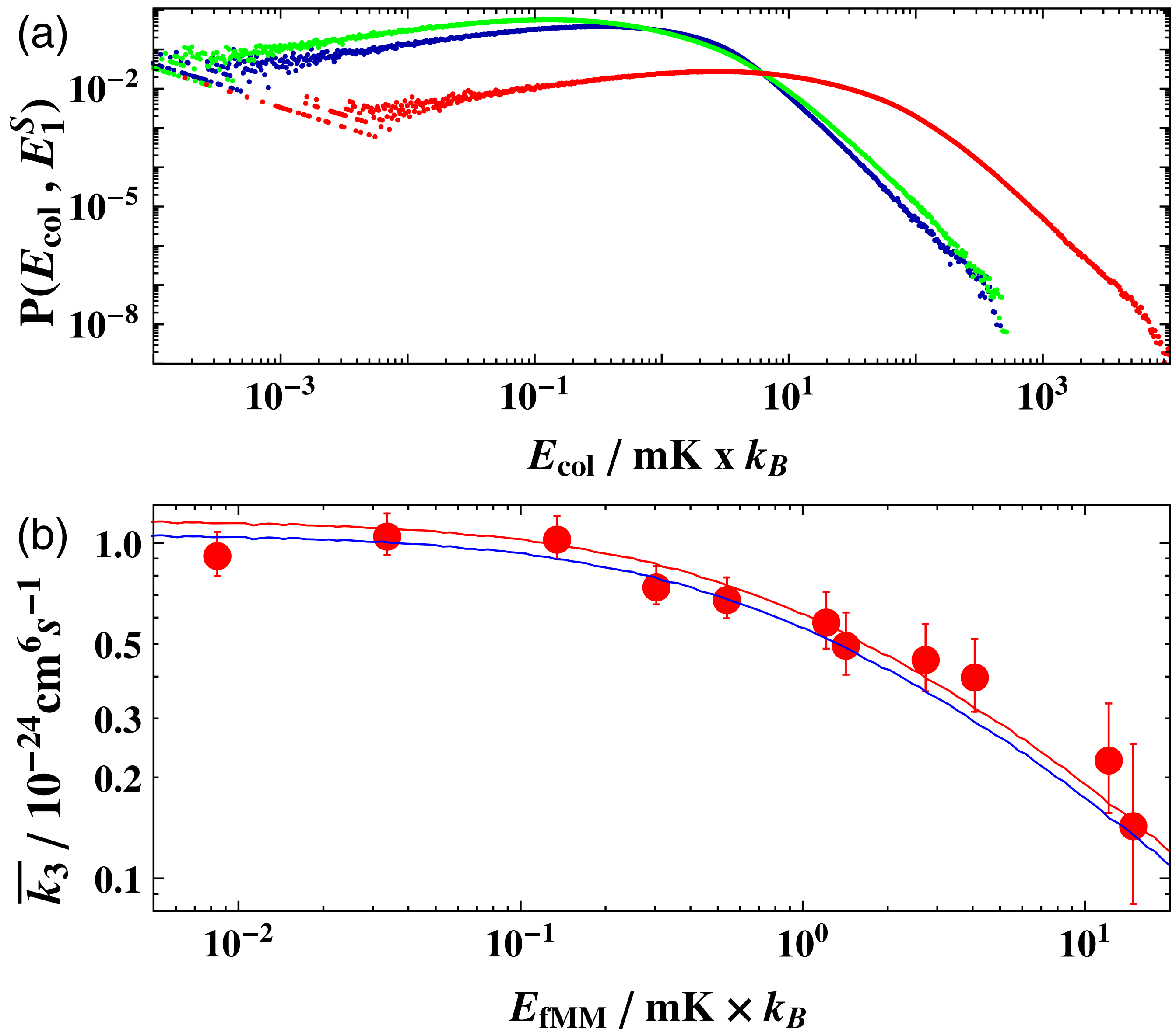
Ion-atom-atom three-body recombination

$Ba^+ + Rb + Rb$

Classical trajectory calculations versus experimental results





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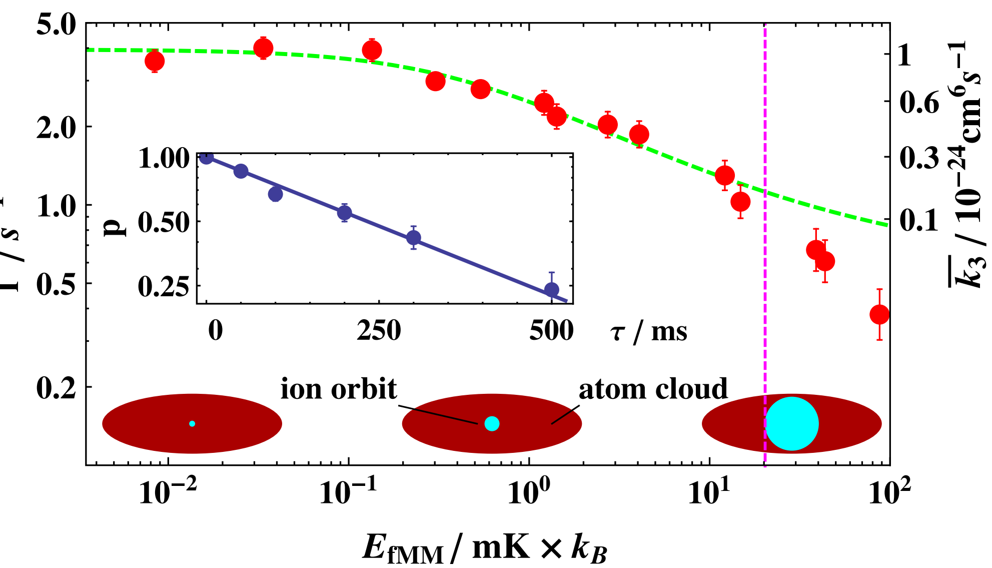
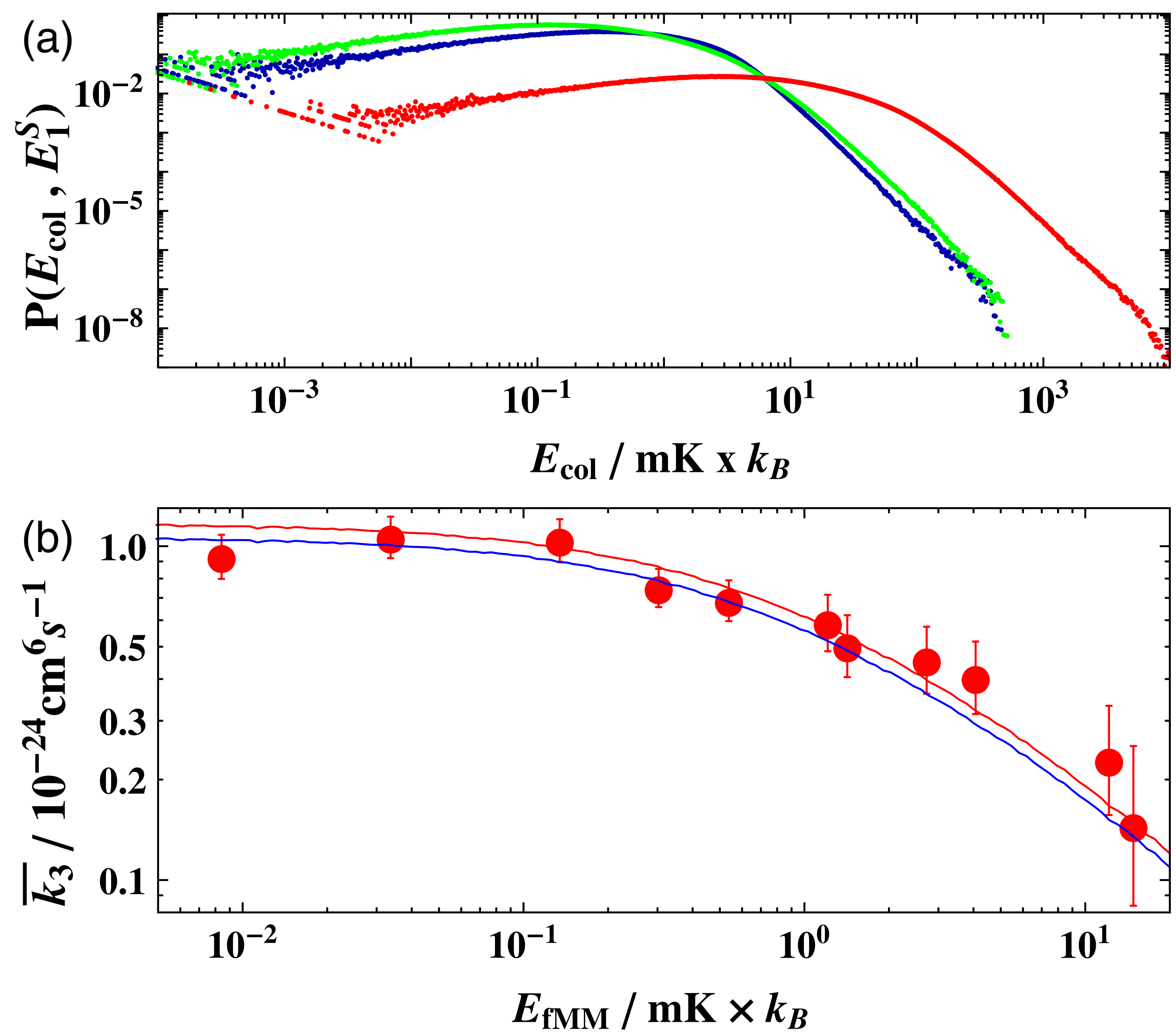




$$\Gamma_3 \sim 10\mathrm{ms}^{-1}$$

A. Krükow et al., PRL **116**, 193201 (2016)

A single ion in a bath of ultracold atoms

Ion-atom-atom three-body recombination

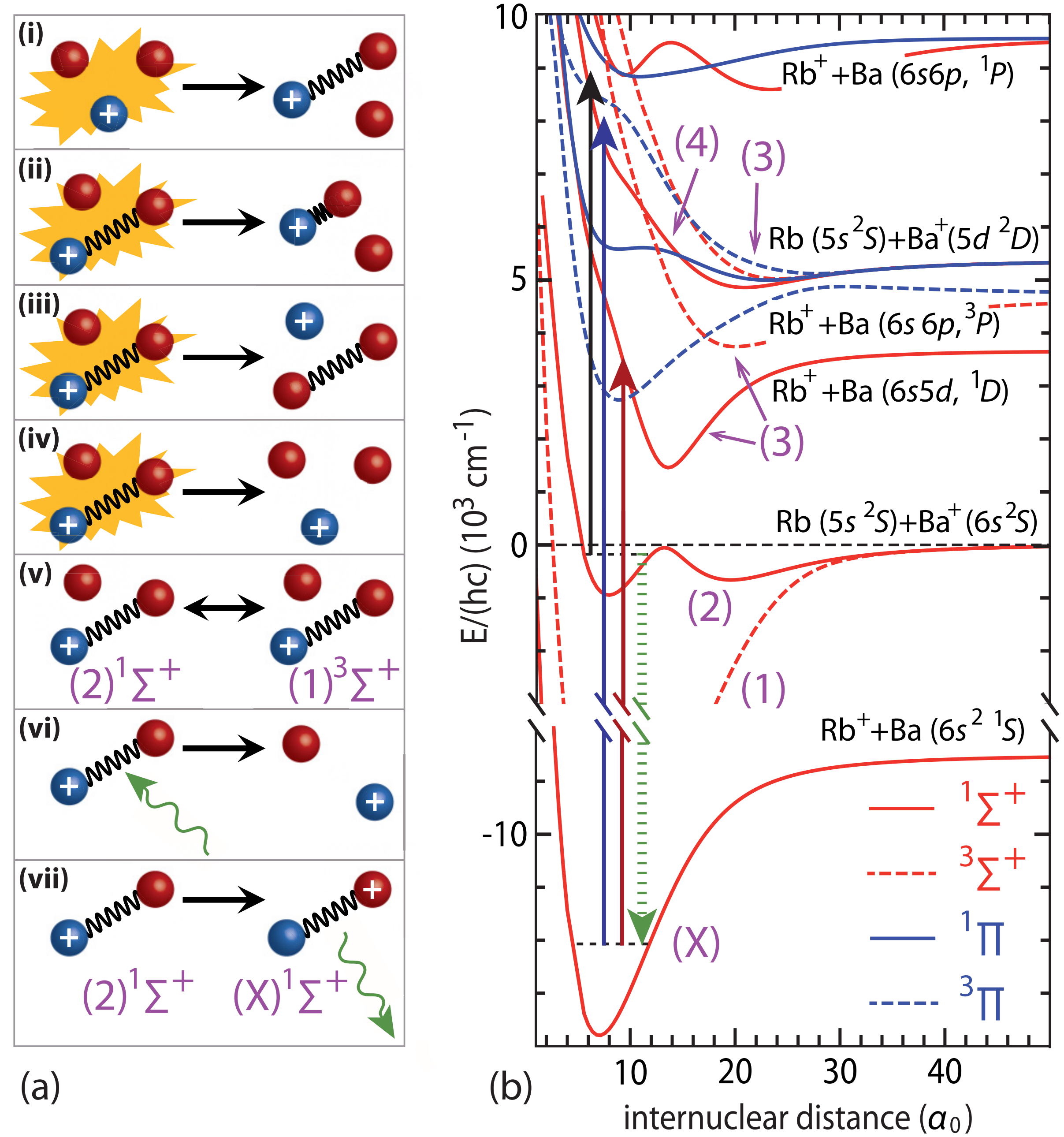
$Ba^+ + Rb + Rb$

PHYSICAL REVIEW RESEARCH **3**, 013196 (2021)

Life and death of a cold $BaRb^+$ molecule inside an ultracold cloud of Rb atoms

Amir Mohammadi,[1] Artjom Krükow,[1] Amir Mahdian,[1] Markus Deiß,[1] Jesús Pérez-Ríos,[2] Humberto da Silva, Jr.,[3] Maurice Raoult,[3] Olivier Dulieu,[3] and Johannes Hecker Denschlag[1,*]

Photodissociation of weakly bound molecular ions



Ion-atom-atom three-body recombination

Threshold behaviour

$$E_k \sim -\frac{C_4}{r^4}$$

J. Pérez-Ríos and C. H. Greene, JCP **143**, 041105 (2015).

A single ion in a bath of ultracold atoms

Ion-atom-atom three-body recombination

Threshold behaviour

$$E_k \sim -\frac{C_4}{r^4} \longrightarrow b_{\max} \sim \left(\frac{C_4}{E_k}\right)^{1/4}$$

J. Pérez-Ríos and C. H. Greene, JCP **143**, 041105 (2015).

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Ion-atom-atom three-body recombination

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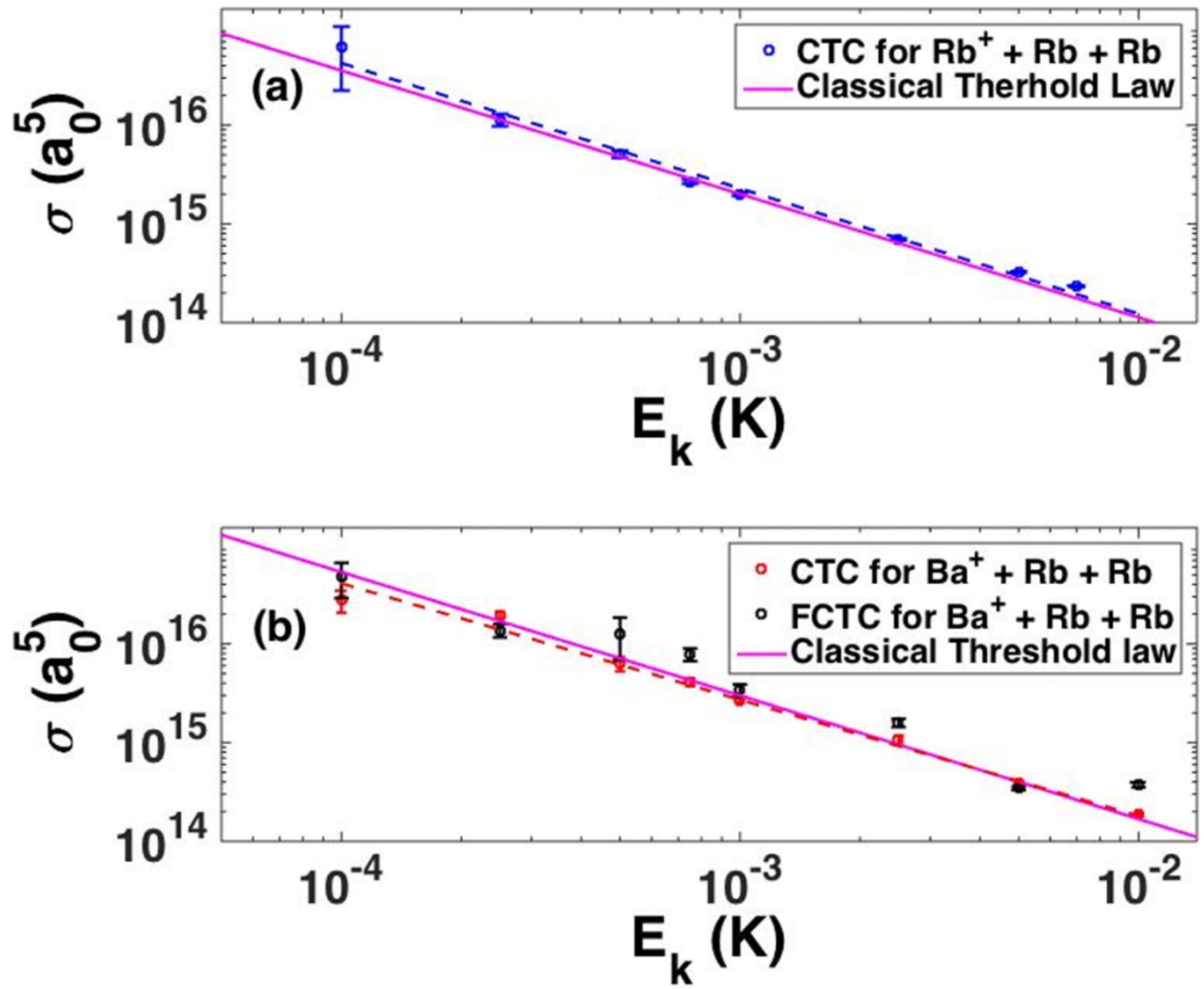

$$\sigma(E_k) \propto E_k^{-5/4}$$

J. Pérez-Ríos and C. H. Greene, JCP **143**, 041105 (2015).

A single ion in a bath of ultracold atoms

Ion-atom-atom three-body recombination

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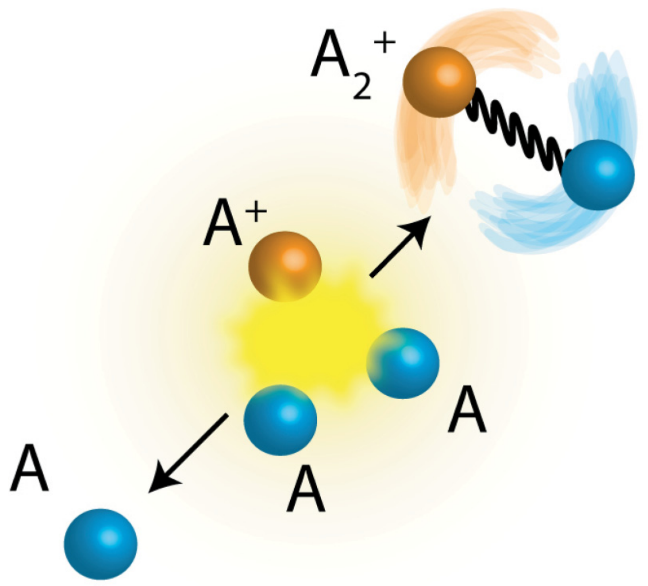
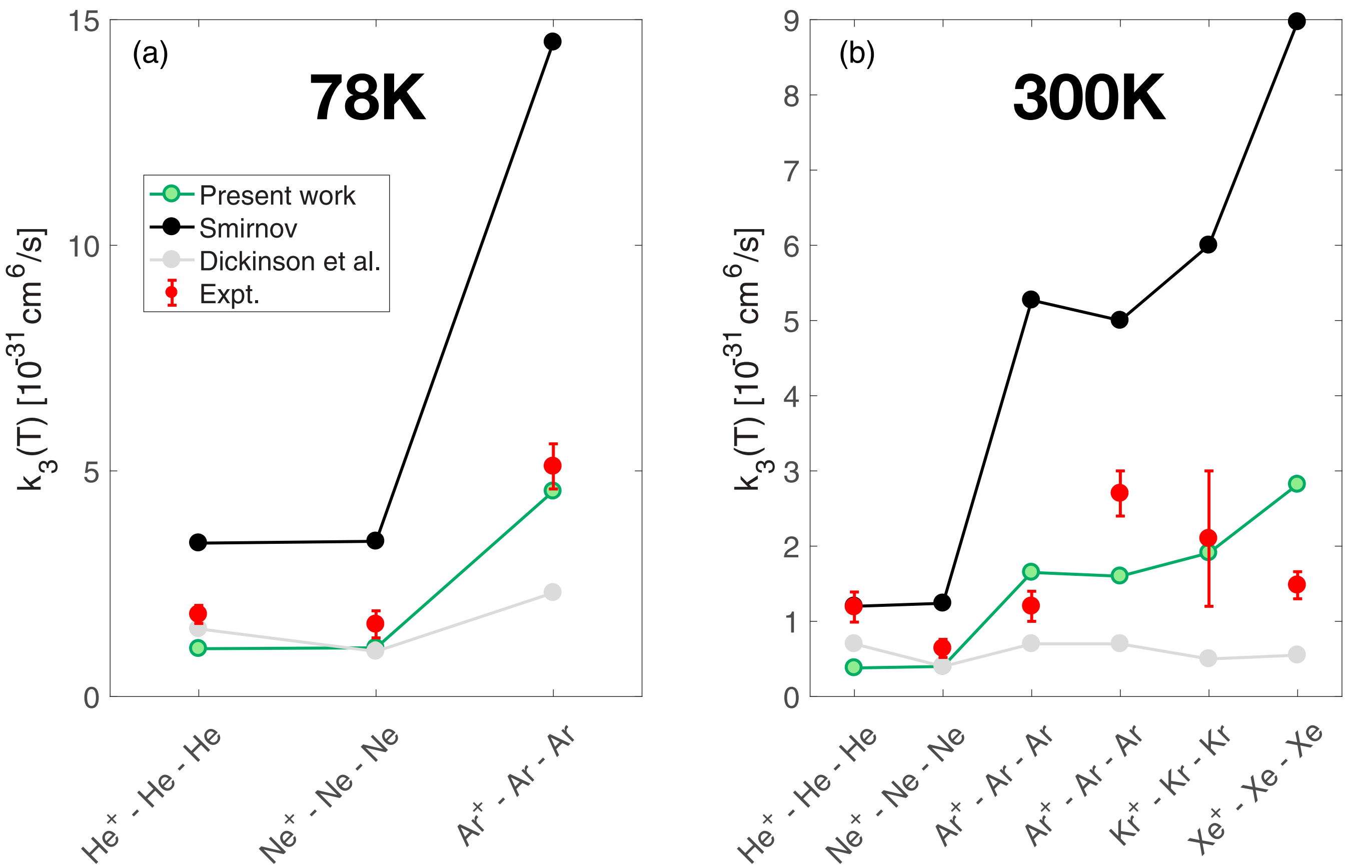


$$A^+ + A + A \rightarrow A_2^+ + A$$
$$\rightarrow A_2 + A^+$$

PHYSICAL REVIEW A **98**, 062707 (2018)

Universal temperature dependence of the ion-neutral-neutral three-body recombination rate

Jesús Pérez-Ríos[1] and Chris H. Greene[2]

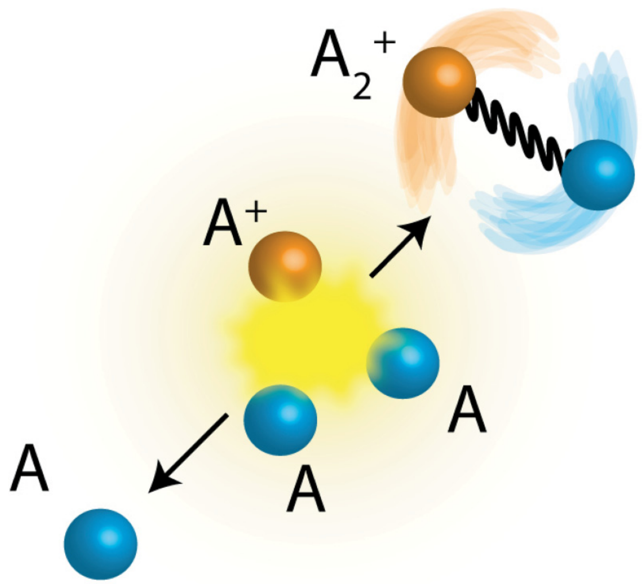


J. Pérez-Ríos and C. H. Greene, JCP **143**, 041105 (2015).

A single ion in a bath of ultracold atoms

Ion-atom-atom three-body recombination

Threshold behaviour



$$A^+ + A + A \rightarrow A_2^+ + A$$

$$\rightarrow A_2 + A^+$$

PHYSICAL REVIEW A **98**, 062707 (2018)

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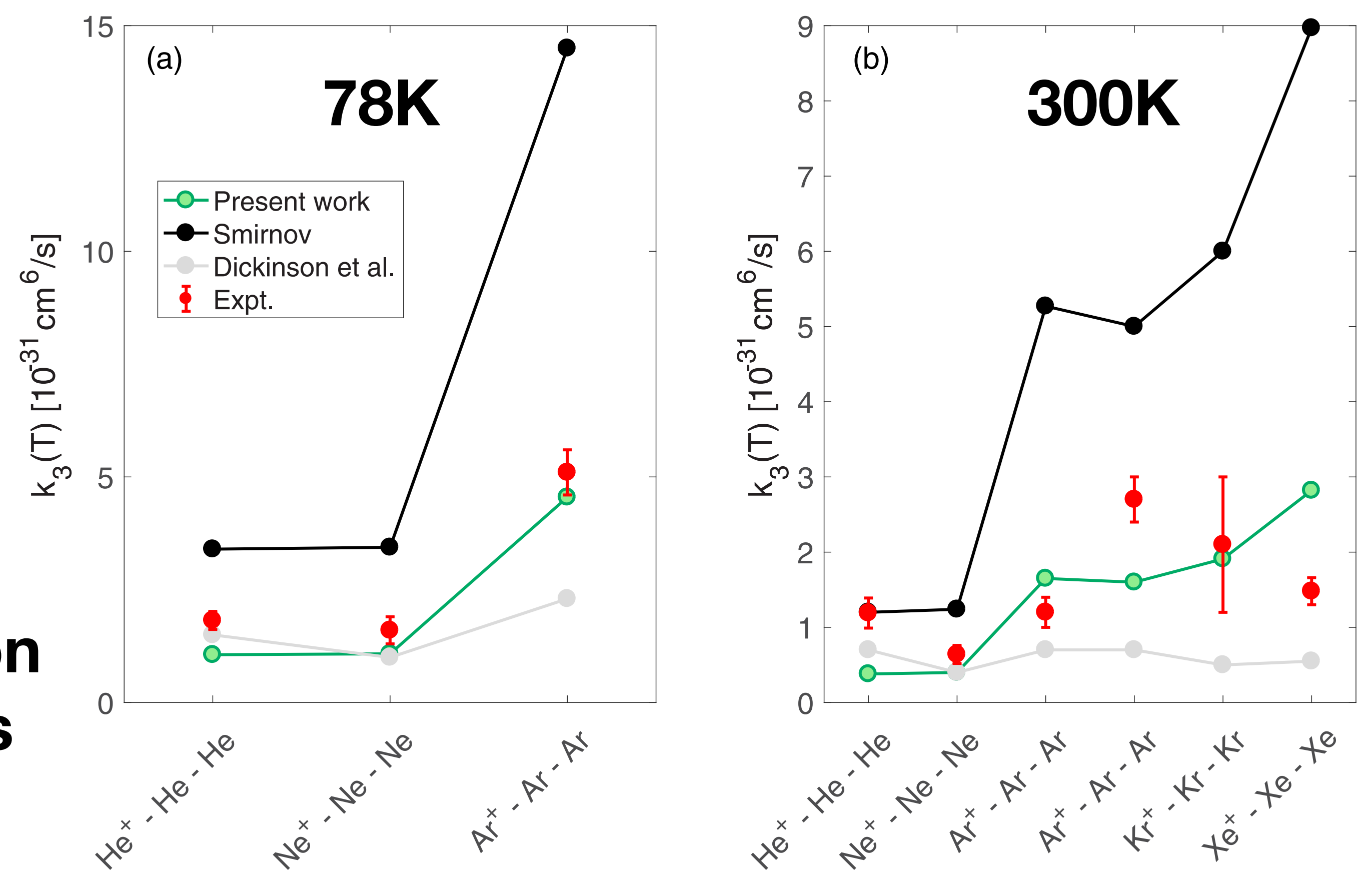

Ion-atom-atom three-body recombination leads to the formation of molecular ions

$$\sigma(E_k) \propto E_k^{-5/4}$$

J. Pérez-Ríos and C. H. Greene, JCP **143**, 041105 (2015).

A single ion in a bath of ultracold molecules

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PHYSICAL REVIEW RESEARCH **2**, 033232 (2020)

Controlling the nature of a charged impurity in a bath of Feshbach dimers

Henrik Hirzler,[1] Eleanor Trimby,[1] Rianne S. Lous,[1] Gerrit C. Groenenboom,[2] Rene Gerritsma,[1]
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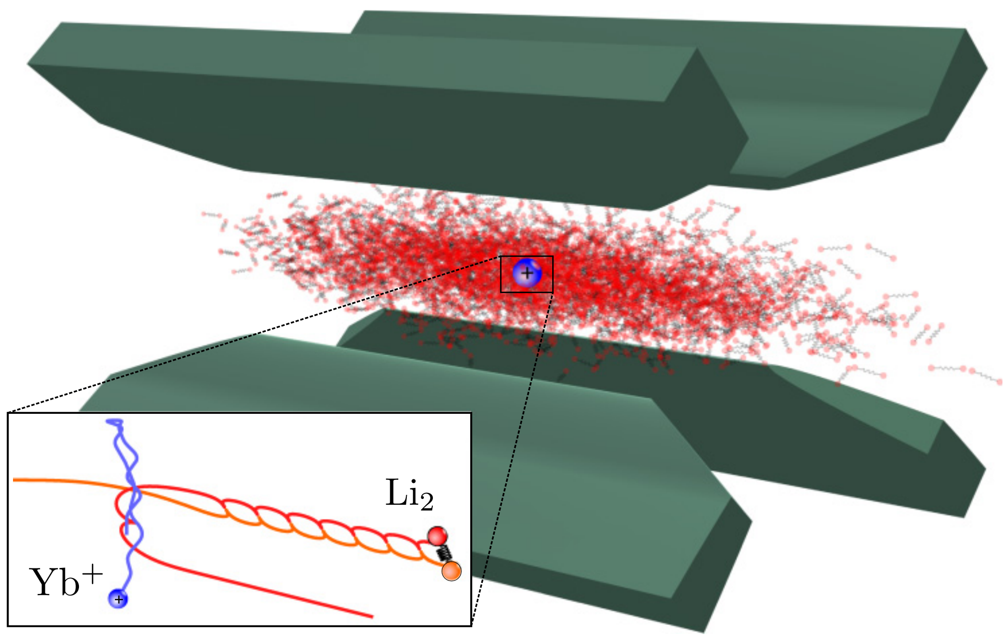

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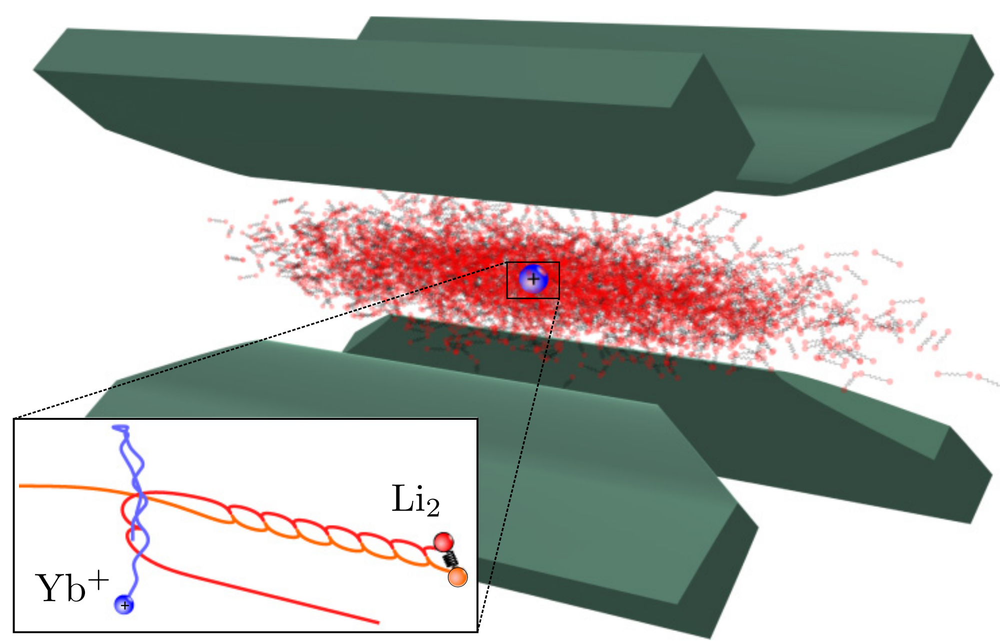

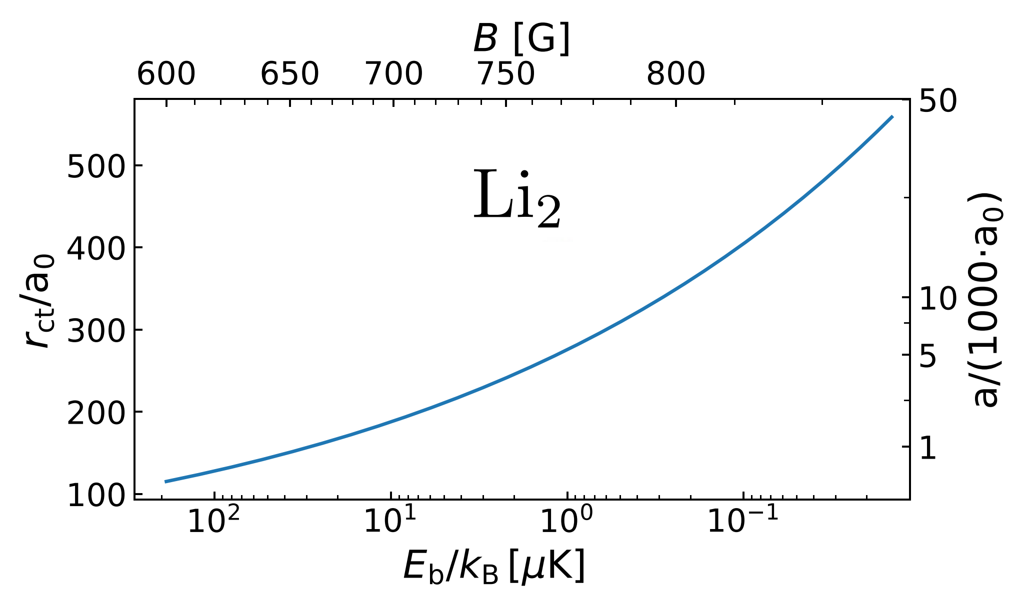

A single ion in a bath of ultracold molecules

Reactive and inelastic processes

PHYSICAL REVIEW RESEARCH **2**, 033232 (2020)

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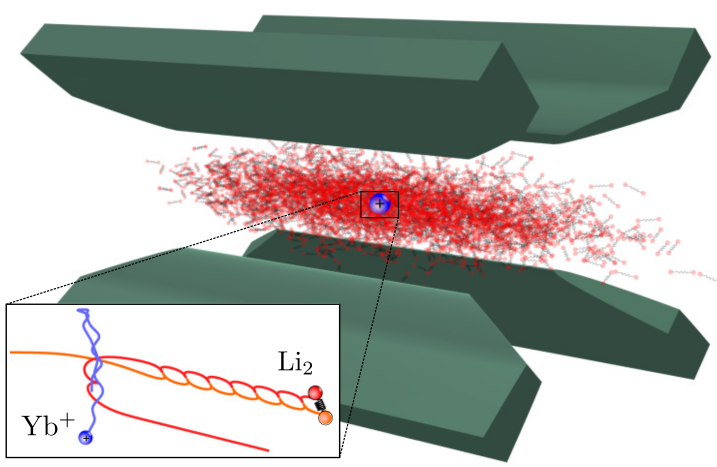
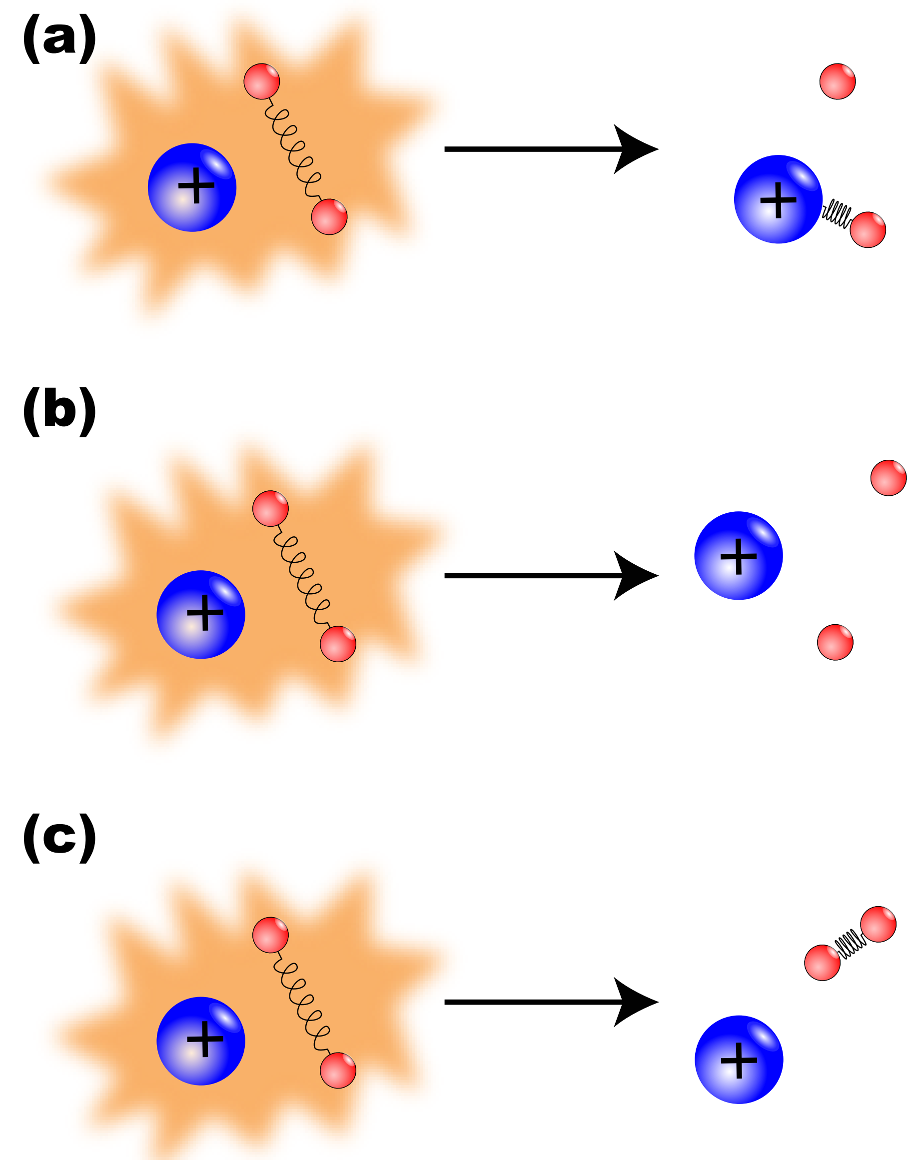


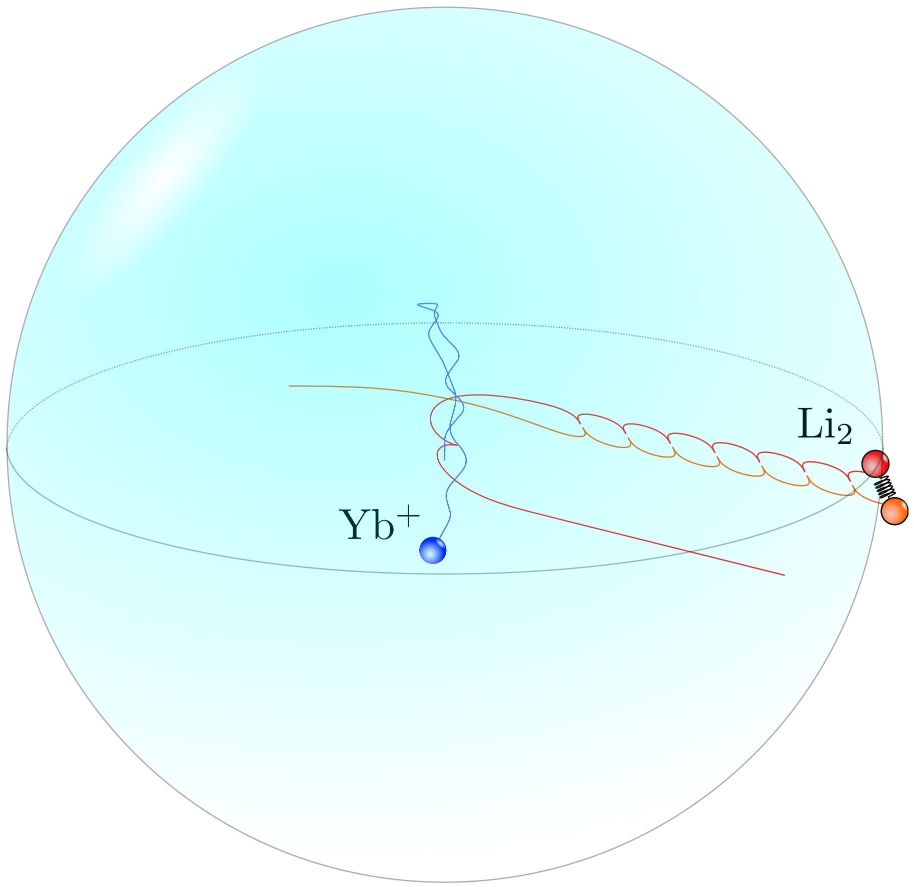


H. Hirzler et al., PRR **2**, 033232 (2020).

Reactive and inelastic processes

Quasi-classical trajectory calculations

$$H = \frac{\boldsymbol{P}_1^2}{2m_{12}} + \frac{\boldsymbol{P}_2^2}{2m_{3,12}} + V(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2).$$



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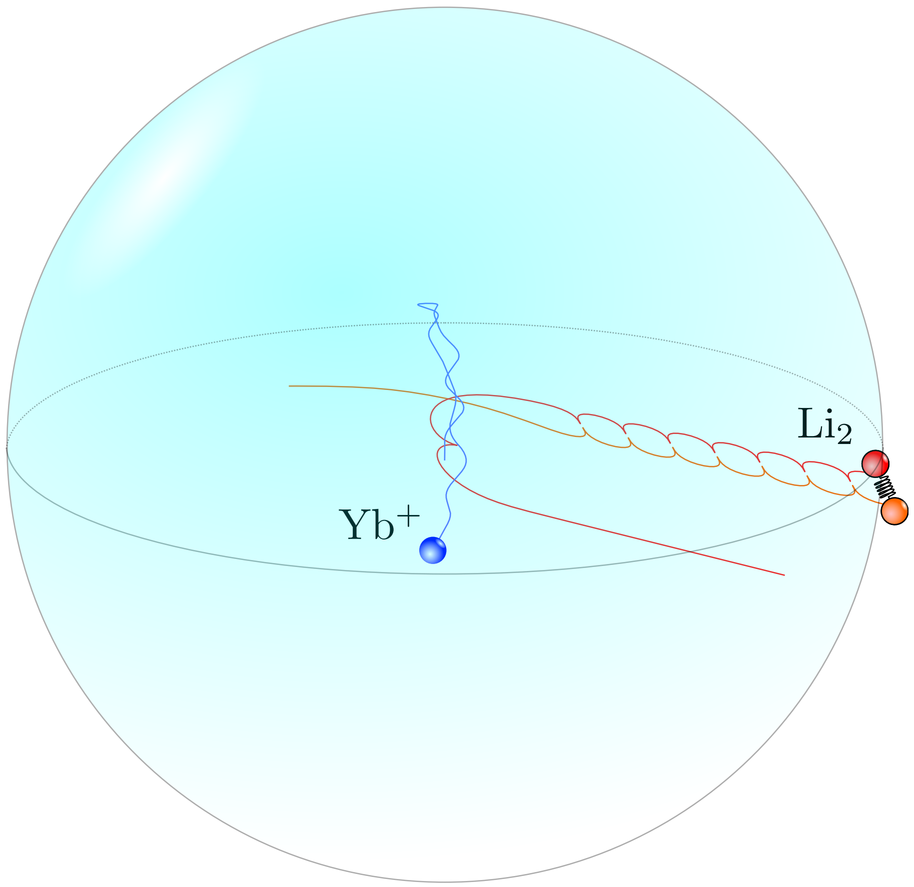
Interartomic potentials

$$V_{\mathrm{ai}}(r_{\mathrm{ai}}) = -\frac{C_4^{\mathrm{ai}}}{2r_{\mathrm{ai}}^4} + \frac{C_6^{\mathrm{ai}}}{r_{\mathrm{ai}}^6}, \quad r_{\mathrm{ai}} = |\vec{r}_{\mathrm{a}} - \vec{r}_{\mathrm{i}}|$$

$$V_{\mathrm{Li}_2}(r_{\mathrm{aa}}) = -\frac{C_6^{\mathrm{aa}}}{r_{\mathrm{aa}}^6} + \frac{C_{12}^{\mathrm{aa}}}{r_{\mathrm{aa}}^{12}}, \quad r_{\mathrm{aa}} = \left|\vec{r}_{\mathrm{a}_1} - \vec{r}_{\mathrm{a}_2}\right|$$



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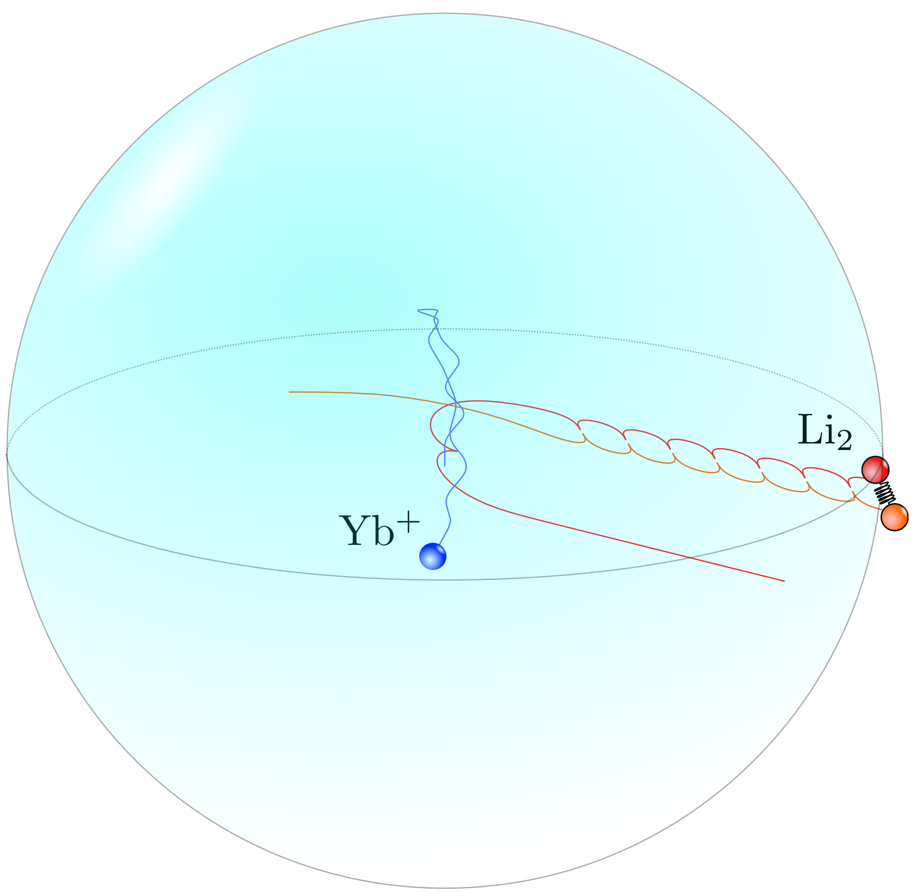
Time-dependent trapping potential

$$V(\vec{r}, t) = \frac{U_{\text{dc}}}{2} \sum_{j=1}^{3} \alpha_j r_{\text{i}_j}^2 + \frac{U_{\text{rf}}}{2} \cos(\Omega t) \sum_{j=1}^{3} \alpha'_j r_{\text{i}_j}^2,$$



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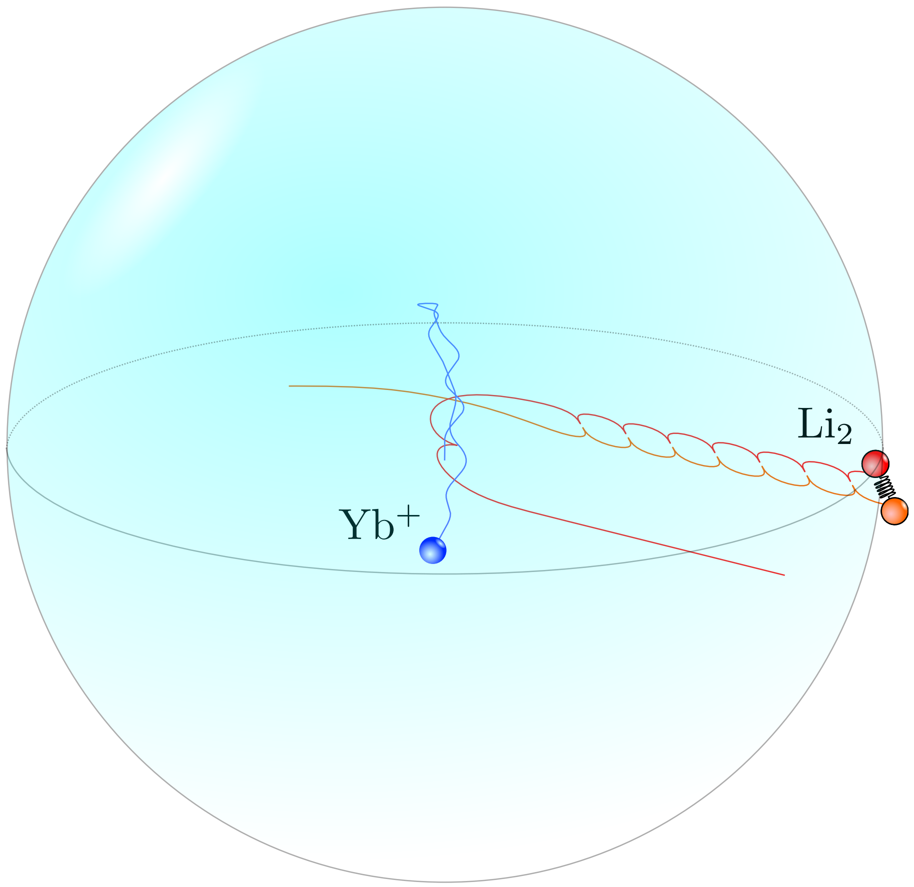
SA



H. Hirzler et al., PRR **2**, 033232 (2020).

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t

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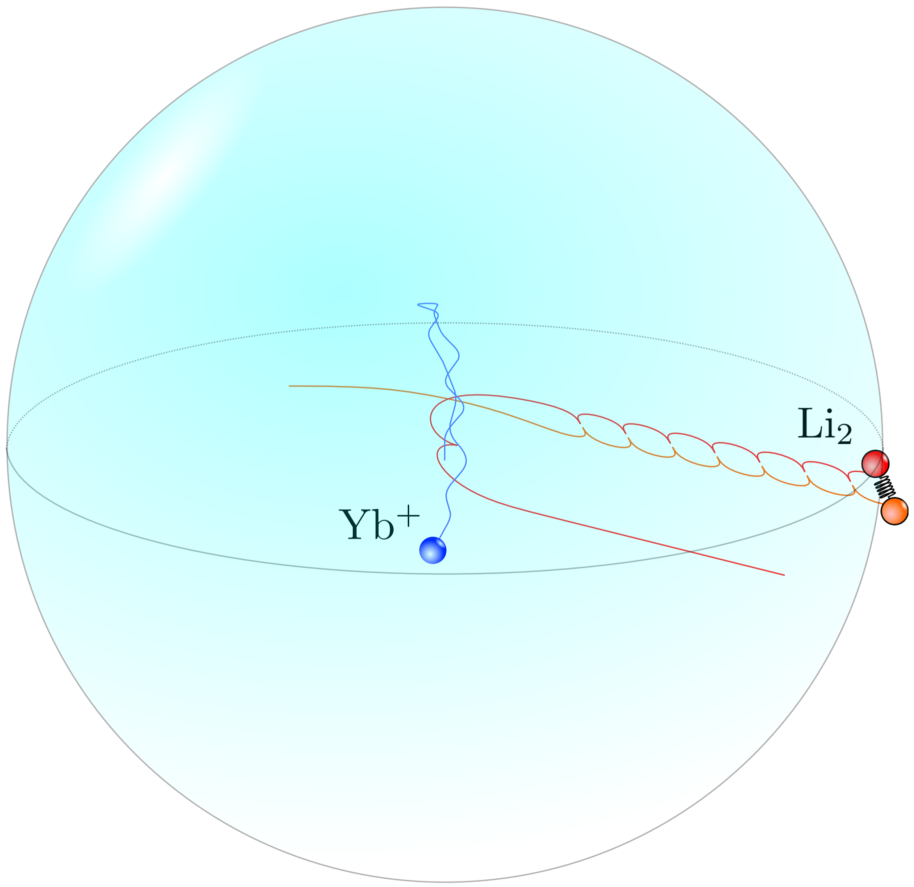
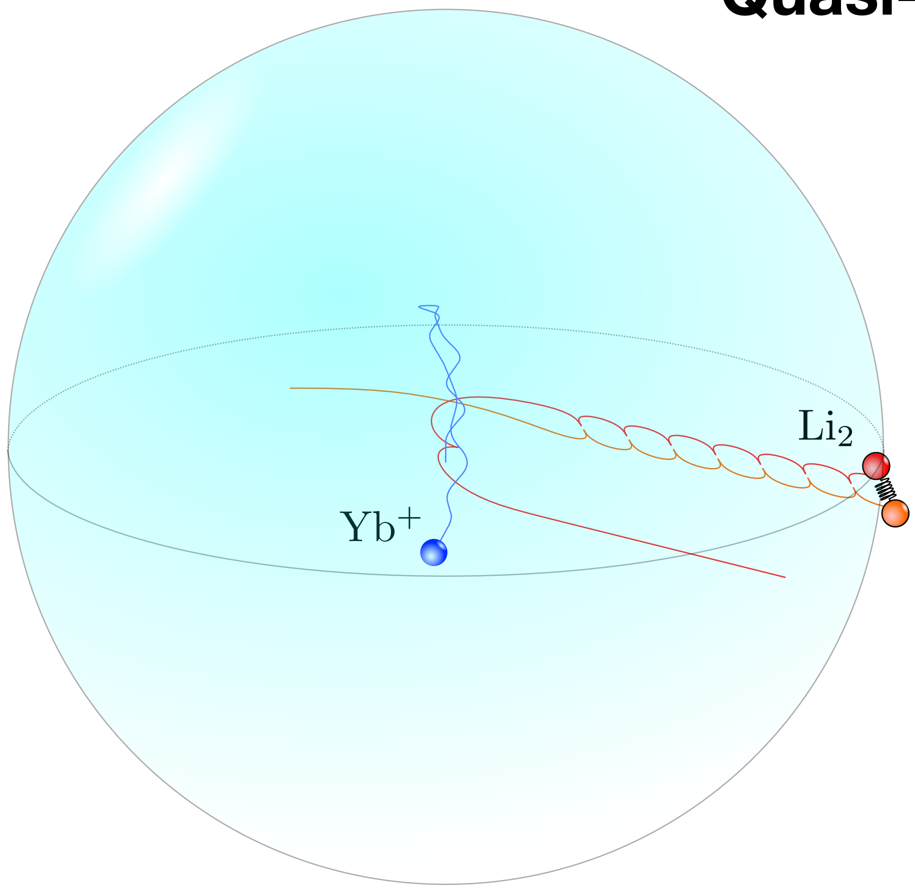


H. Hirzler et al., PRR **2**, 033232 (2020).

A weakly bound molecular ion in a bath of ultracold atoms



Quasi-classical trajectory calculations

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Initial conditions

$$P_1 = \frac{\hbar j(j+1)}{r_+}$$

Final states: from classical phase-space to quantum states through WKB

$$v' = -\frac{1}{2} + \frac{1}{\pi\hbar}\int_{r_-}^{r_+} \sqrt{2m_{12}\left[E_{int} - V(r) - \frac{\hbar^2 j'(j'+1)}{2m_{12}r^2}\right]}dr,$$

J. Pérez-Ríos, PRA **99**, 022707 (2019)

A single ion in a bath of ultracold molecules

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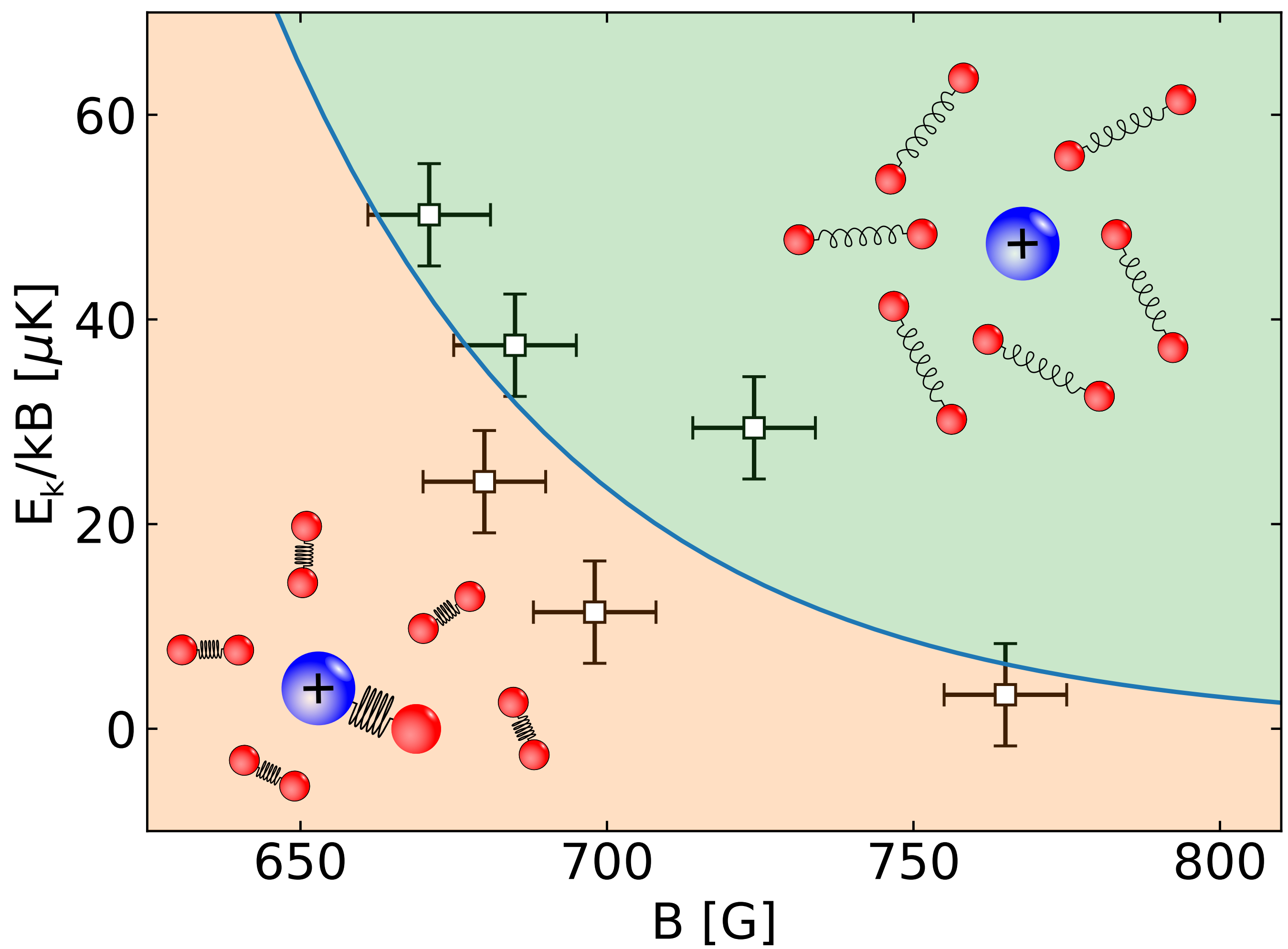
Reactive and inelastic processes

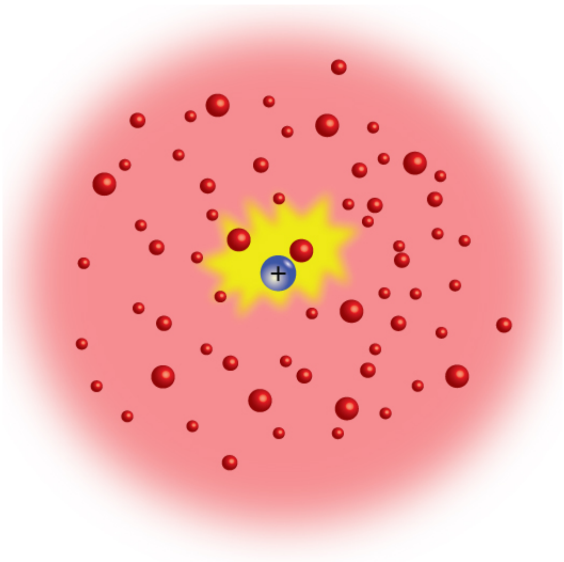
The “phase-diagram” of a charged impurity in a molecular bath



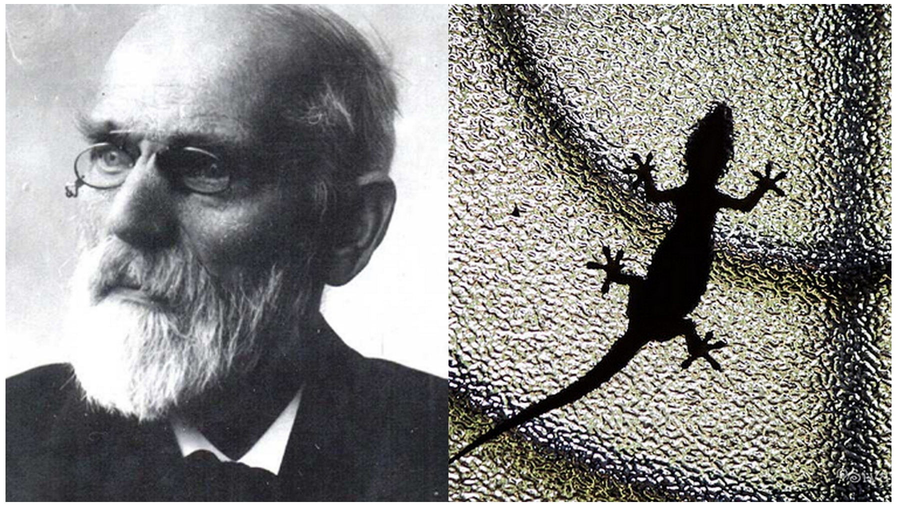
H. Hirzler et al., PRR **2**, 033232 (2020).

Outlook

A single ion in an ultracold bath



Formation of van der Waals molecules



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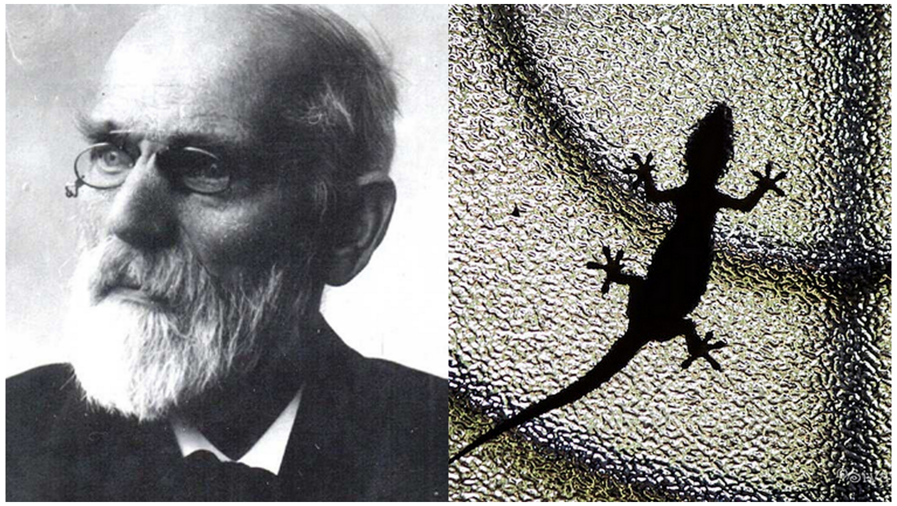
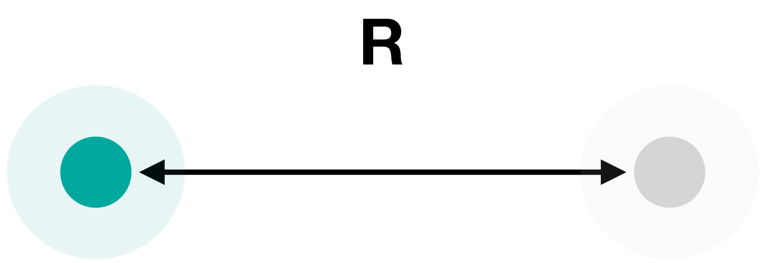


Formation of van der Waals molecules

What are van der Waals molecules?

“Van der Waals molecules are weakly bound complexes of small atoms or molecules held together, not by chemical bonds, but by intermolecular attractions”.

Binding energy ~10cm^{-1}



B. L. Blaney and G. E. Erwing, Annu. Rev. Phys. Chem. **27**, 553 (1976)

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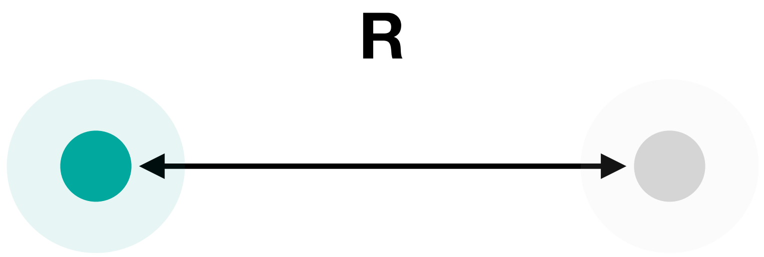

$$V(R) = -\frac{C_6}{R^6}$$

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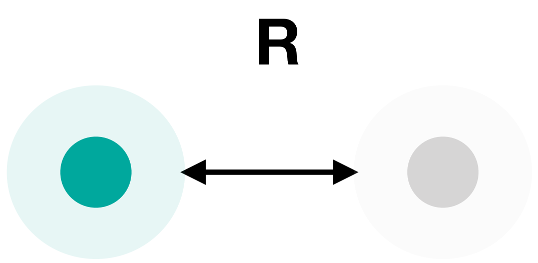

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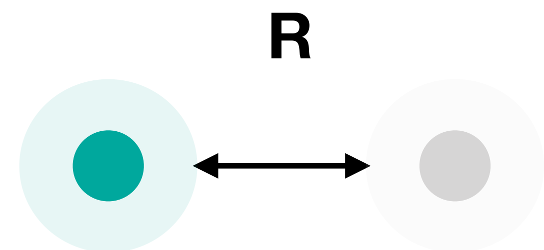

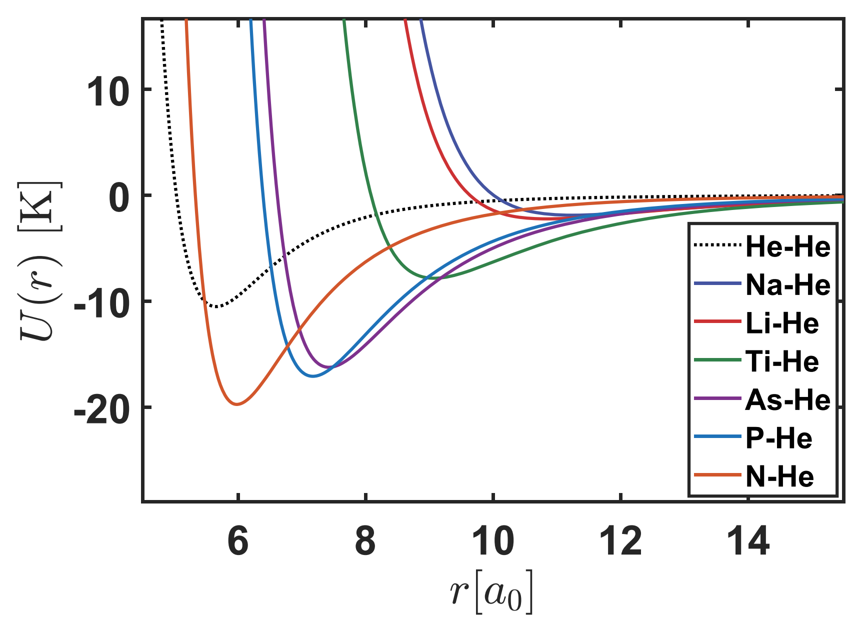

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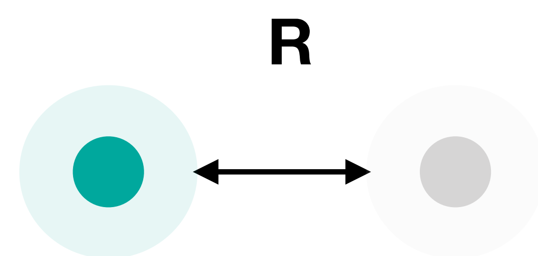
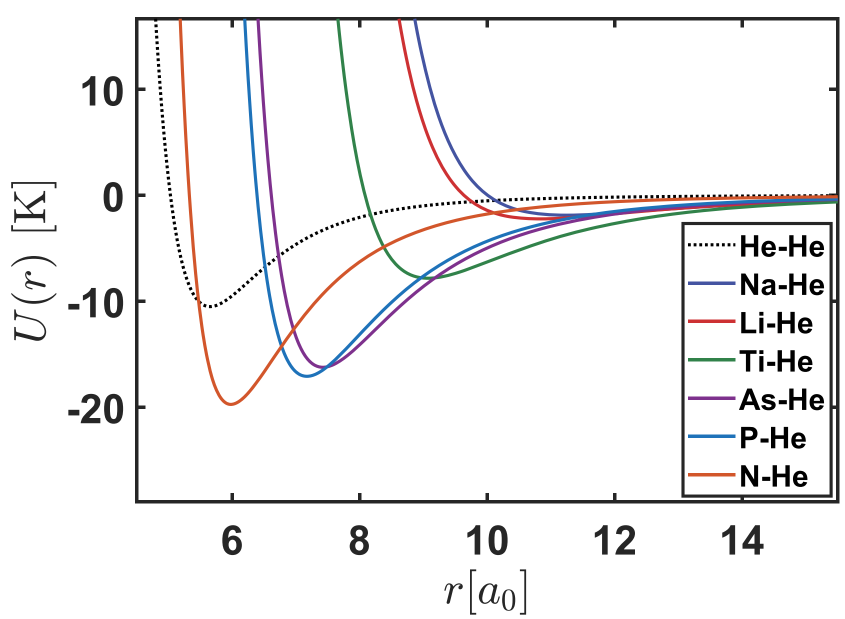
Zn_2



Cd_2



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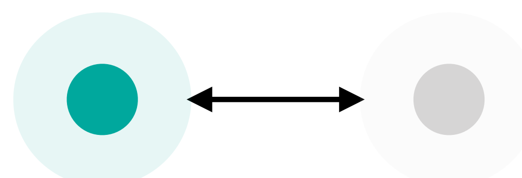
Zn_2

R

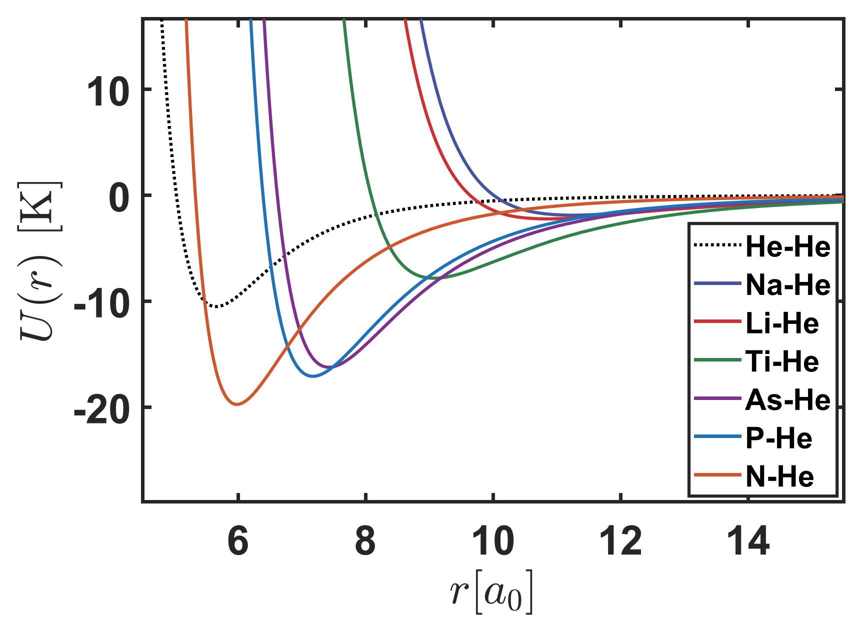


Rare gas atom

Rg-X

Any atom

Cd_2



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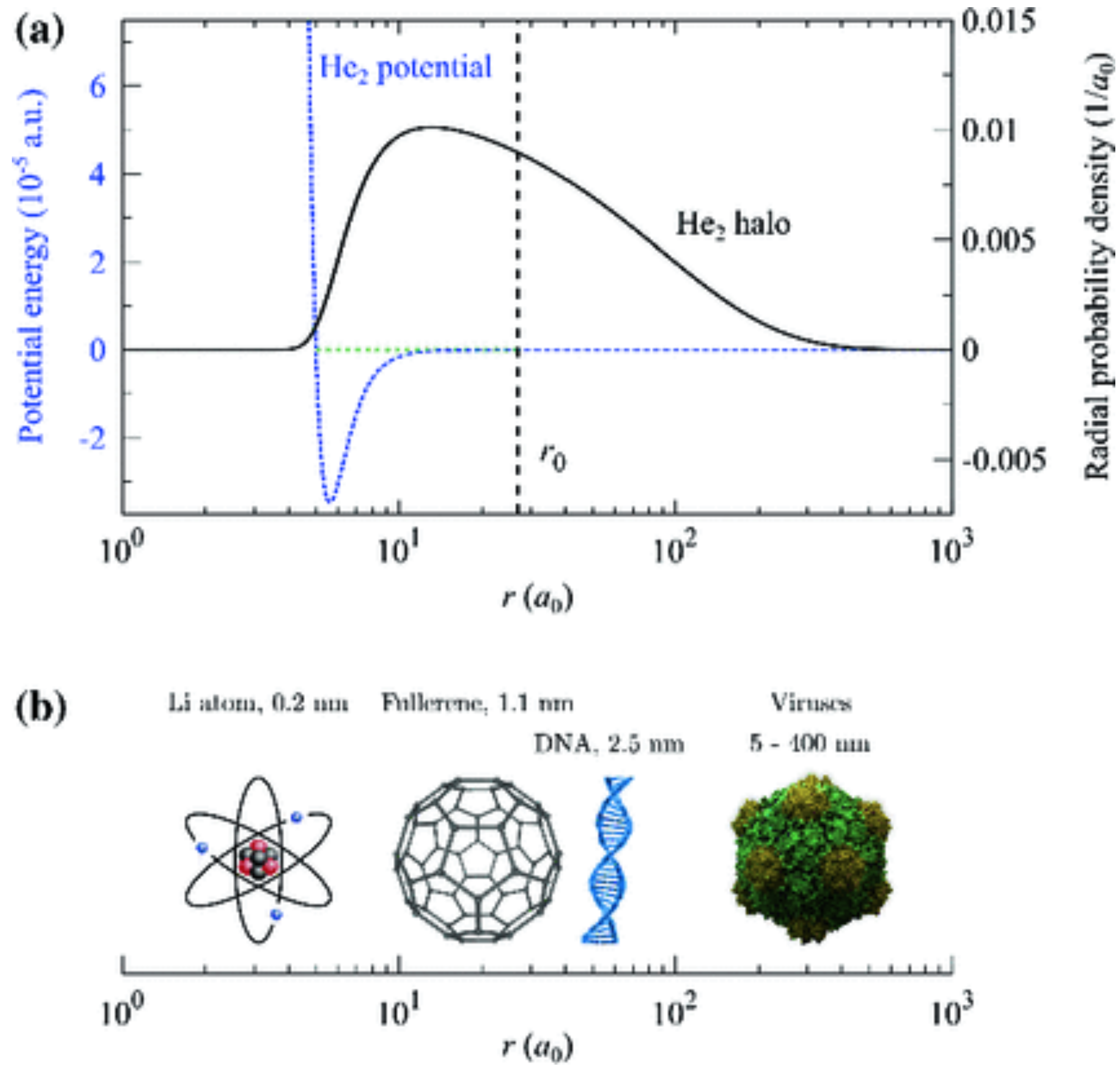
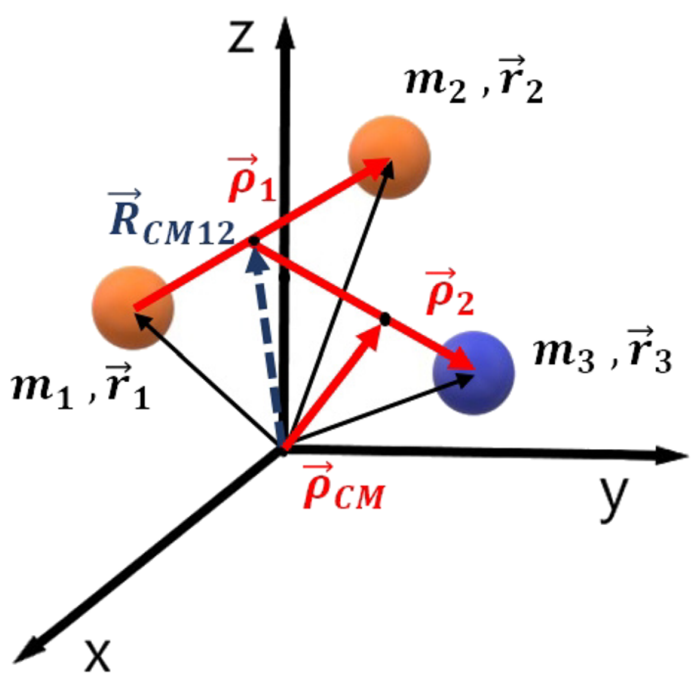
He_2

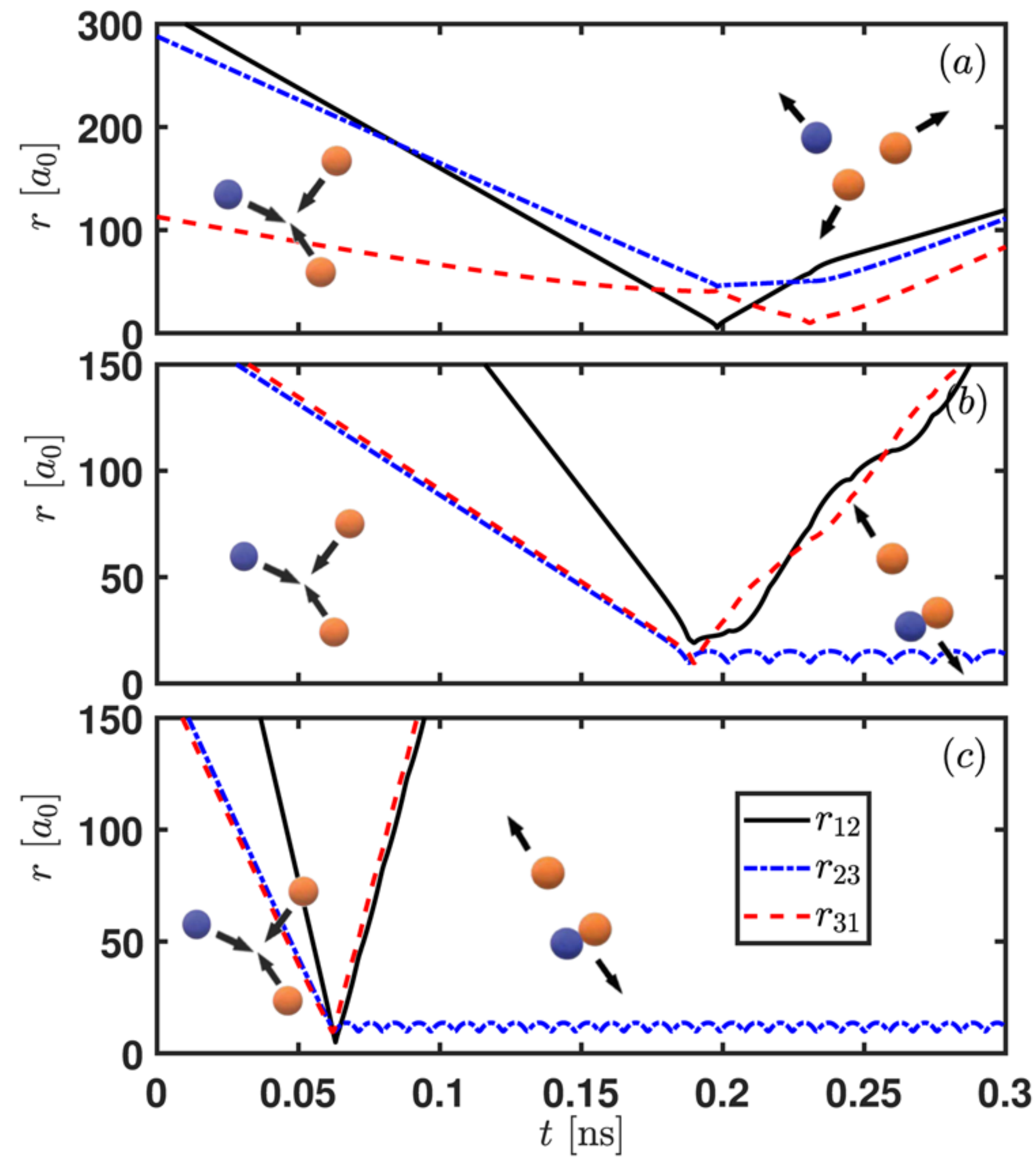


J. Ulmanis Ph.D. thesis (2017)

Formation of van der Waals molecules

Three-body recombination





M. Mirahmadi and J. Pérez-Ríos JCP **154**, 034305 (2021).

Formation of van der Waals molecules

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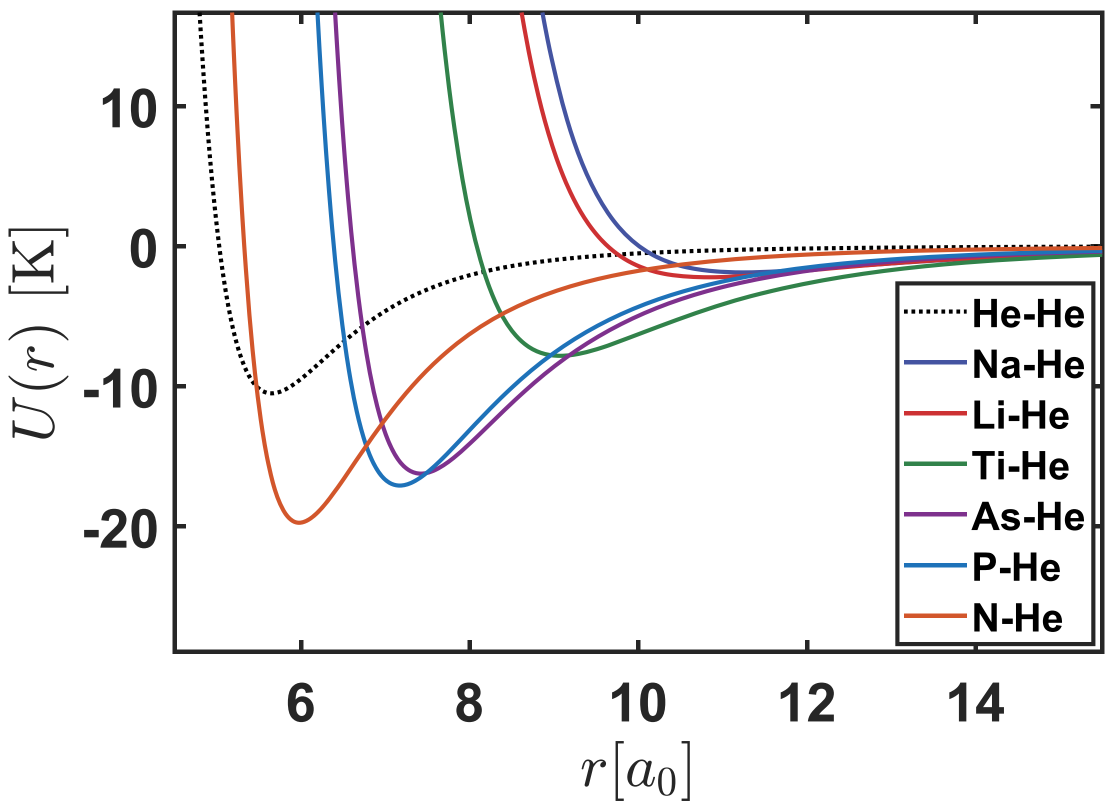

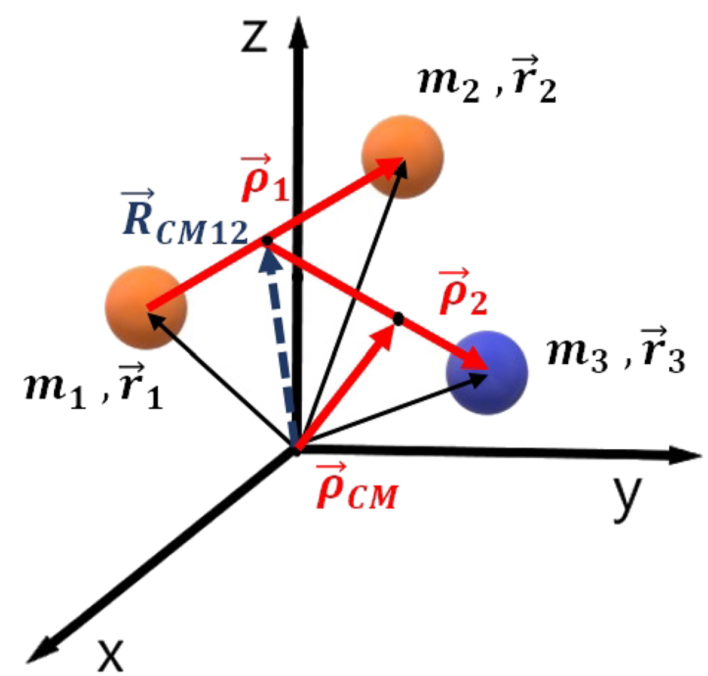

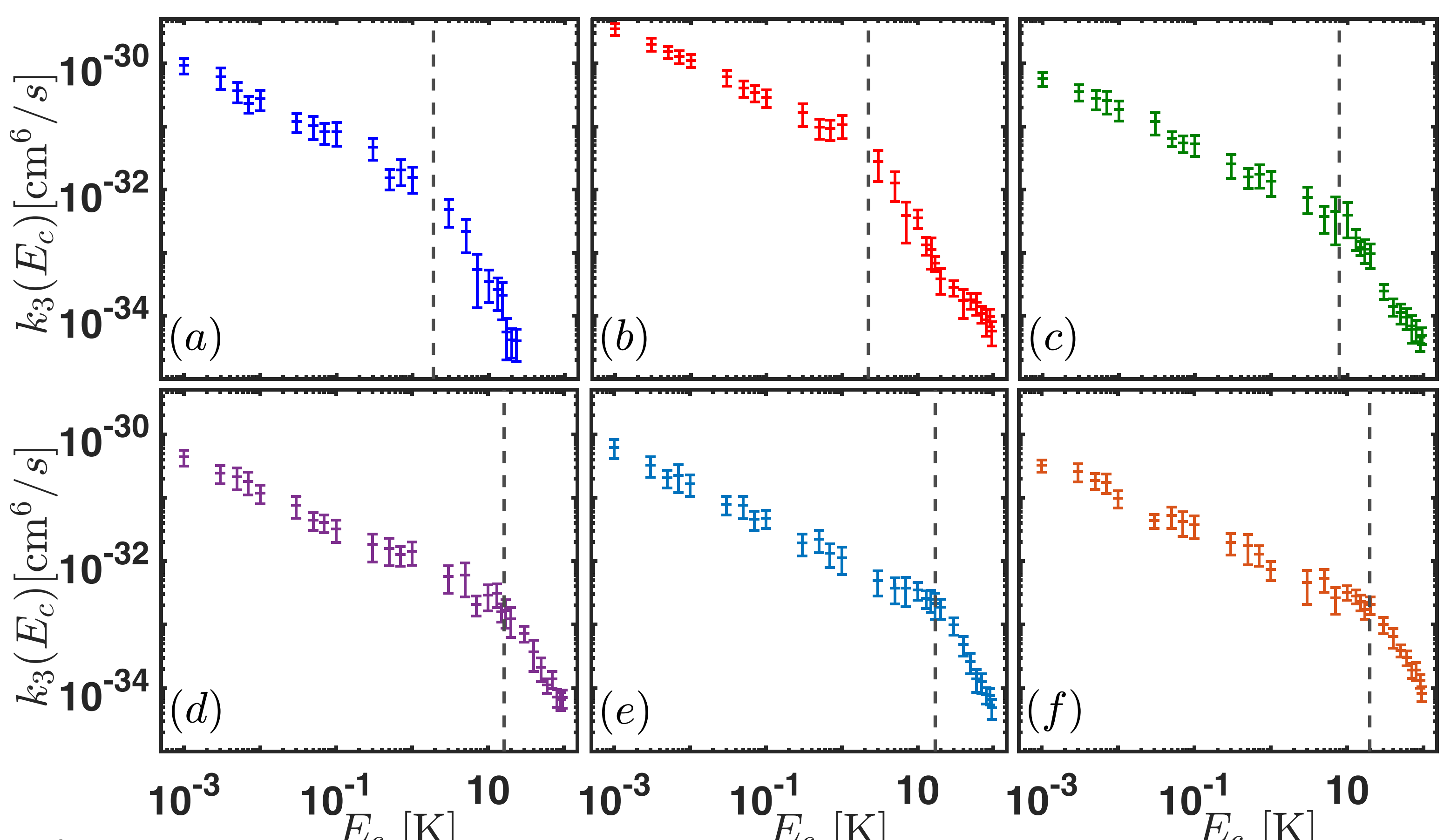

M. Mirahmadi and J. Pérez-Ríos JCP **154**, 034305 (2021).

Formation of van der Waals molecules

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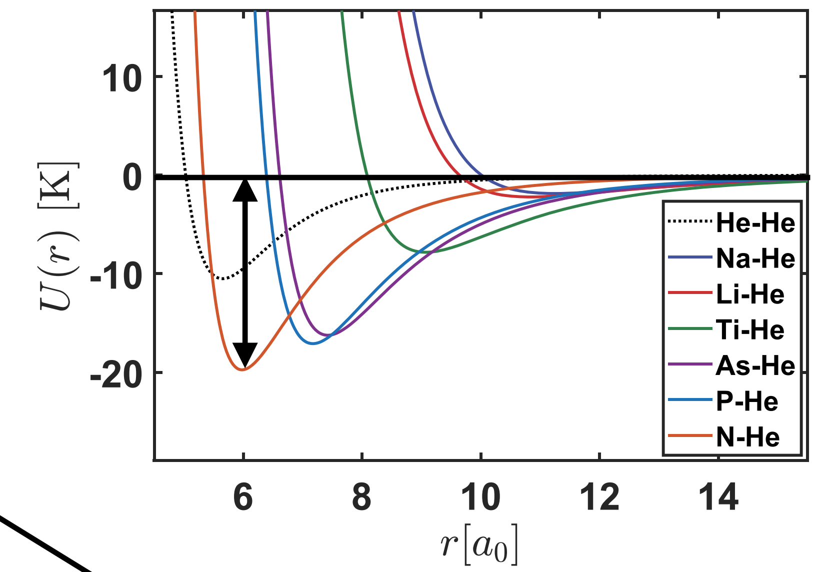
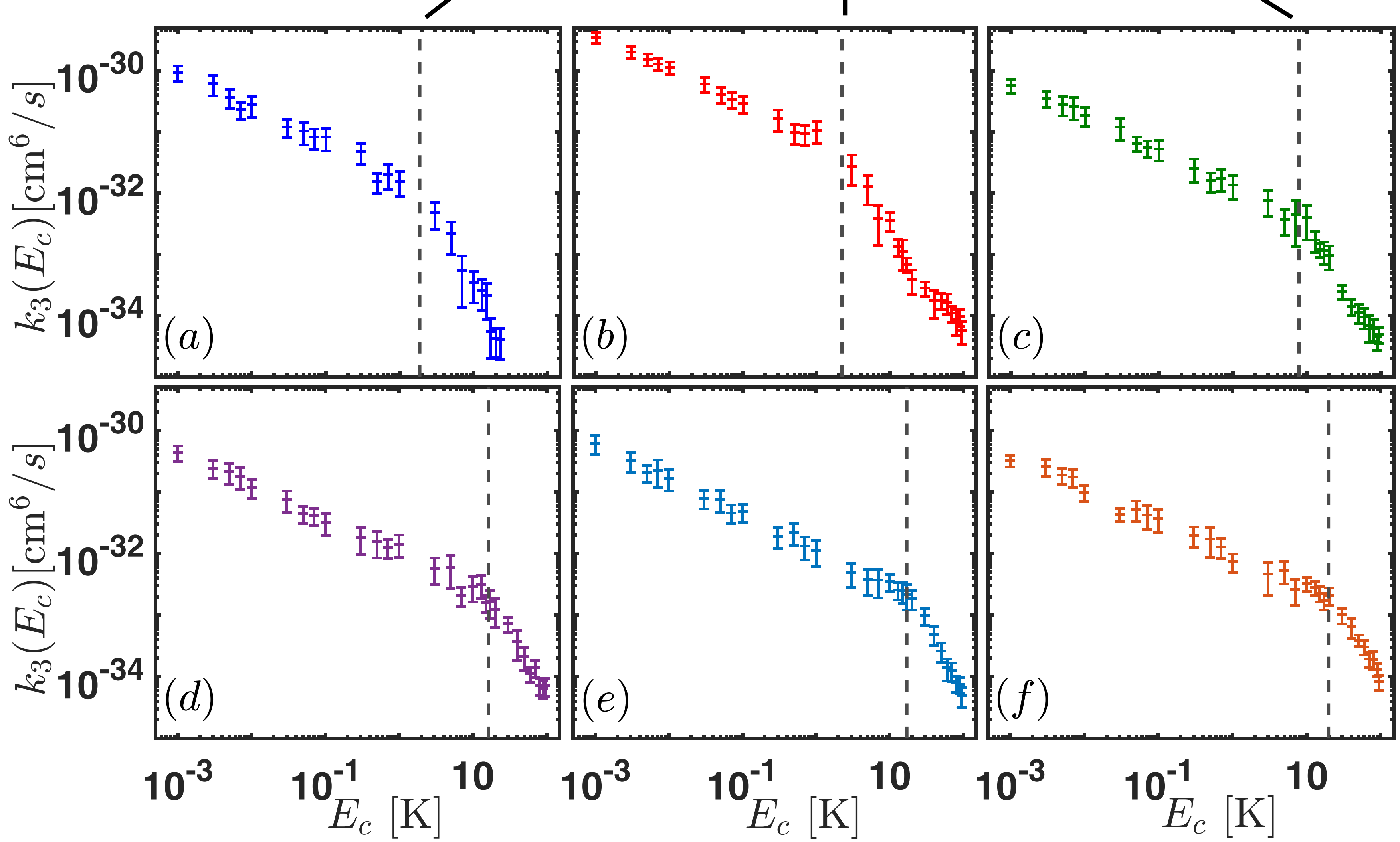


D_e(X-RG)

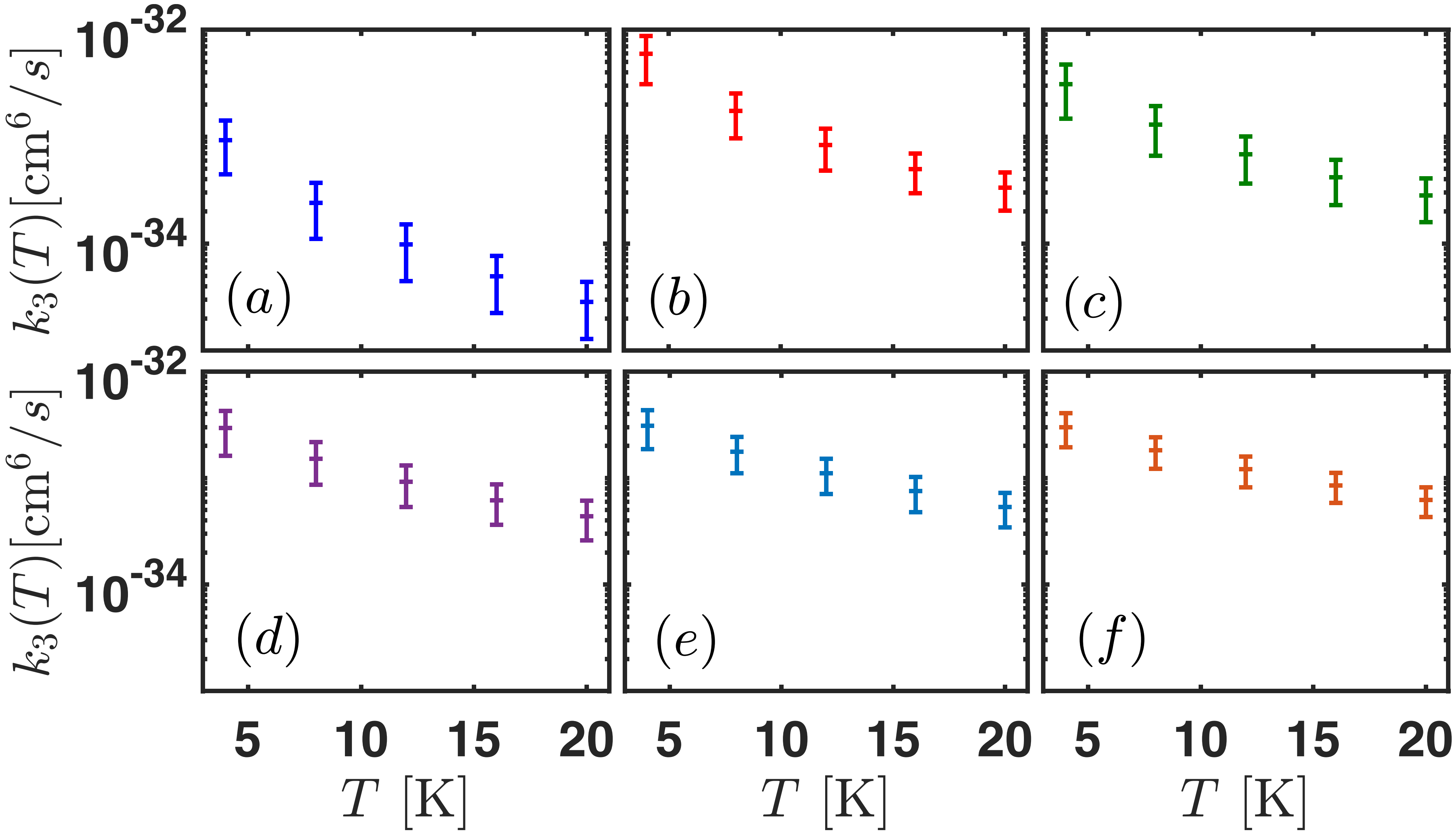


M. Mirahmadi and J. Pérez-Ríos JCP **154**, 034305 (2021).

Formation of van der Waals molecules

What are van der Waals molecules?

Same order of magnitude !!!!

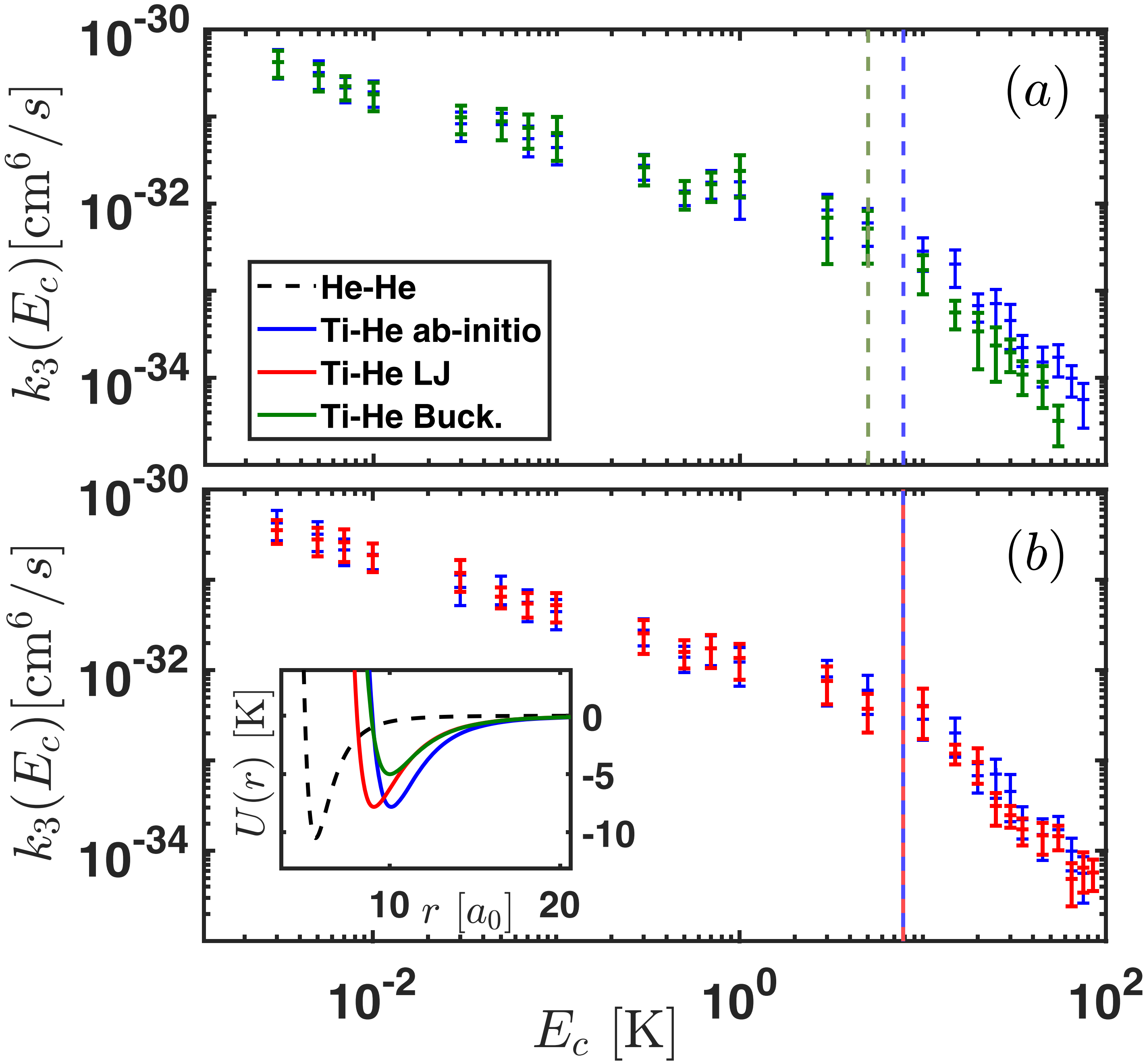


Every atom in a buffer gas will lead to the formation of van der Waals molecules

M. Mirahmadi and J. Pérez-Ríos JCP **154**, 034305 (2021).

Formation of van der Waals molecules

The role of short-range physics



M. Mirahmadi and J. Pérez-Ríos JCP **154**, 034305 (2021).

Concluding remarks

Few-body processes (cold chemistry) play a relevant role on impurity physics

A single ion evolves into a molecular ion in an atomic or molecular gas

Van der Waals molecules emerge as a consequence of three-body recombination

Any atom in a buffer gas source may form a van der Waals molecule

Acknowledgements

Thanks to the organisers specially to Dr. Sourav Dutta for this opportunity

Thank you so much for your attention!!!!!

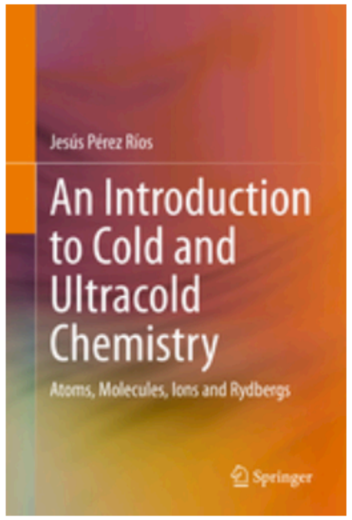
Institute for
Molecules and Materials
Radboud University

More information

If you are interested in learning more please contact me @ jperezri@fhi-berlin.mpg.de

Website: **https://www.fhi.mpg.de/209391/AMO_theory**

» Chemistry » Physical Chemistry



An Introduction to Cold and Ultracold Chemistry

Atoms, Molecules, Ions and Rydbergs

Authors: **Pérez Ríos**, Jesús

Provides readers with an overview of the fundamentals in cold and ultracold chemistry

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