Многомасштабное моделирование матрично-изолированных систем

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доцент Химического факультета МГУ

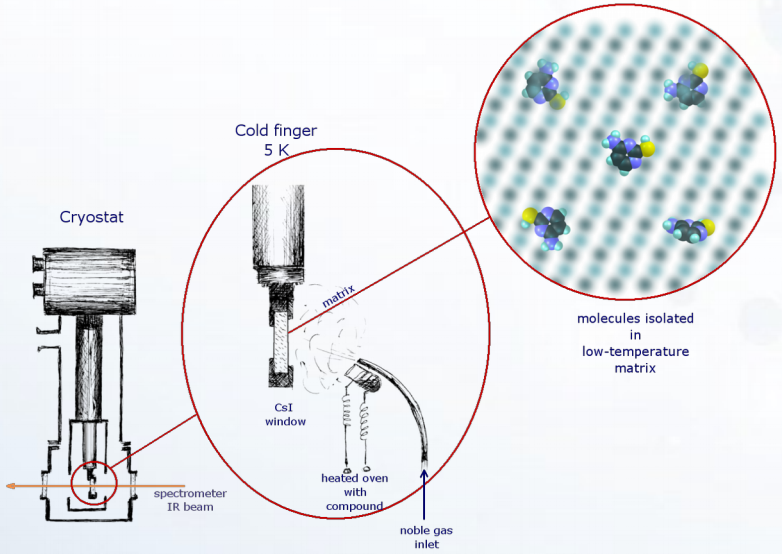
старший научный сотрудник Сколтеха

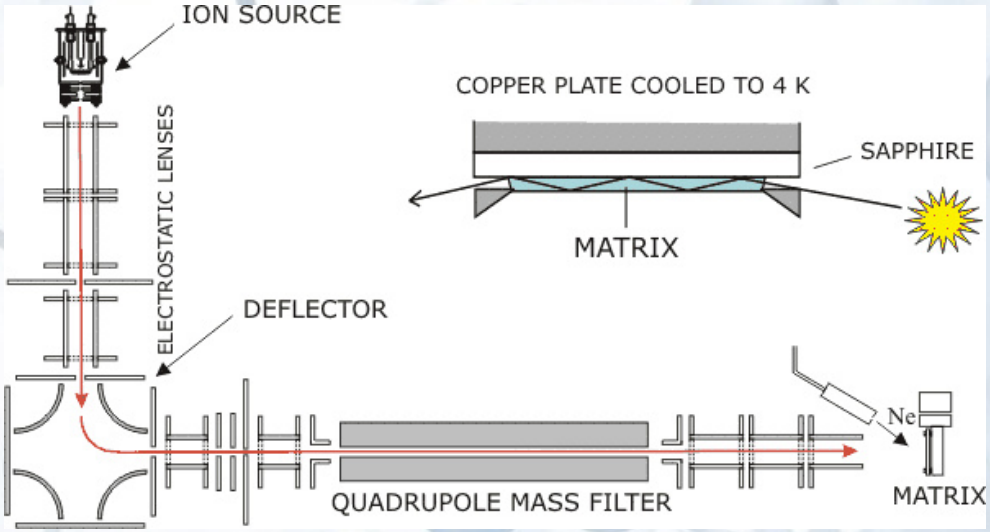
Семинар “Суперкомпьютерные технологии в науке, образовании и промышленности”
НОЦ "Суперкомпьютерные технологии", МГУ Москва, 21 мая 2019.

Матричная изоляция: цели и задачи (эксп)

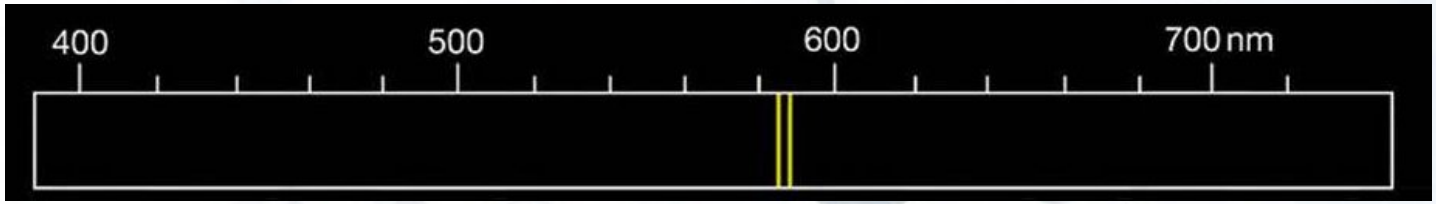
"In the study of free radicals and other unstable substances, an inherent difficulty is the maintenance of a suitable concentration... The intent of the [matrix isolation] method is to trap active molecules in a solid matrix of inert material, crystalline or glassy... The active material can be produced in a variety of ways: by chemical reaction involving two reactants, by pyrolysis, by dissociation in a glow discharge or an arc, or by photolysis."

E. Whittle, D.A. Dows, and G. C. Pimentel, J. Chem. Phys. 22 (1954) 1943





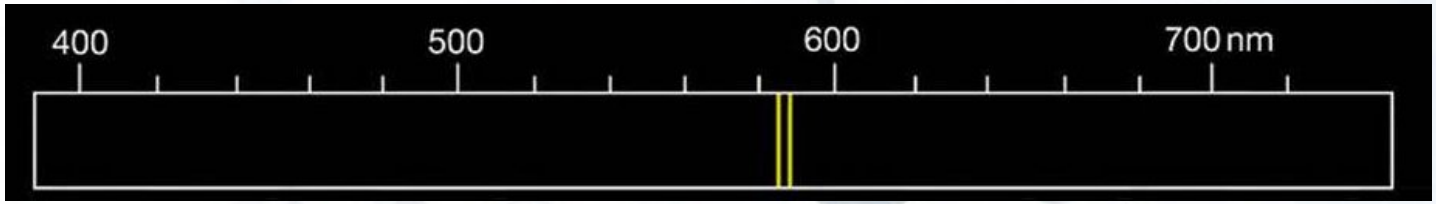
Матричная изоляция: проблемы (эксп)

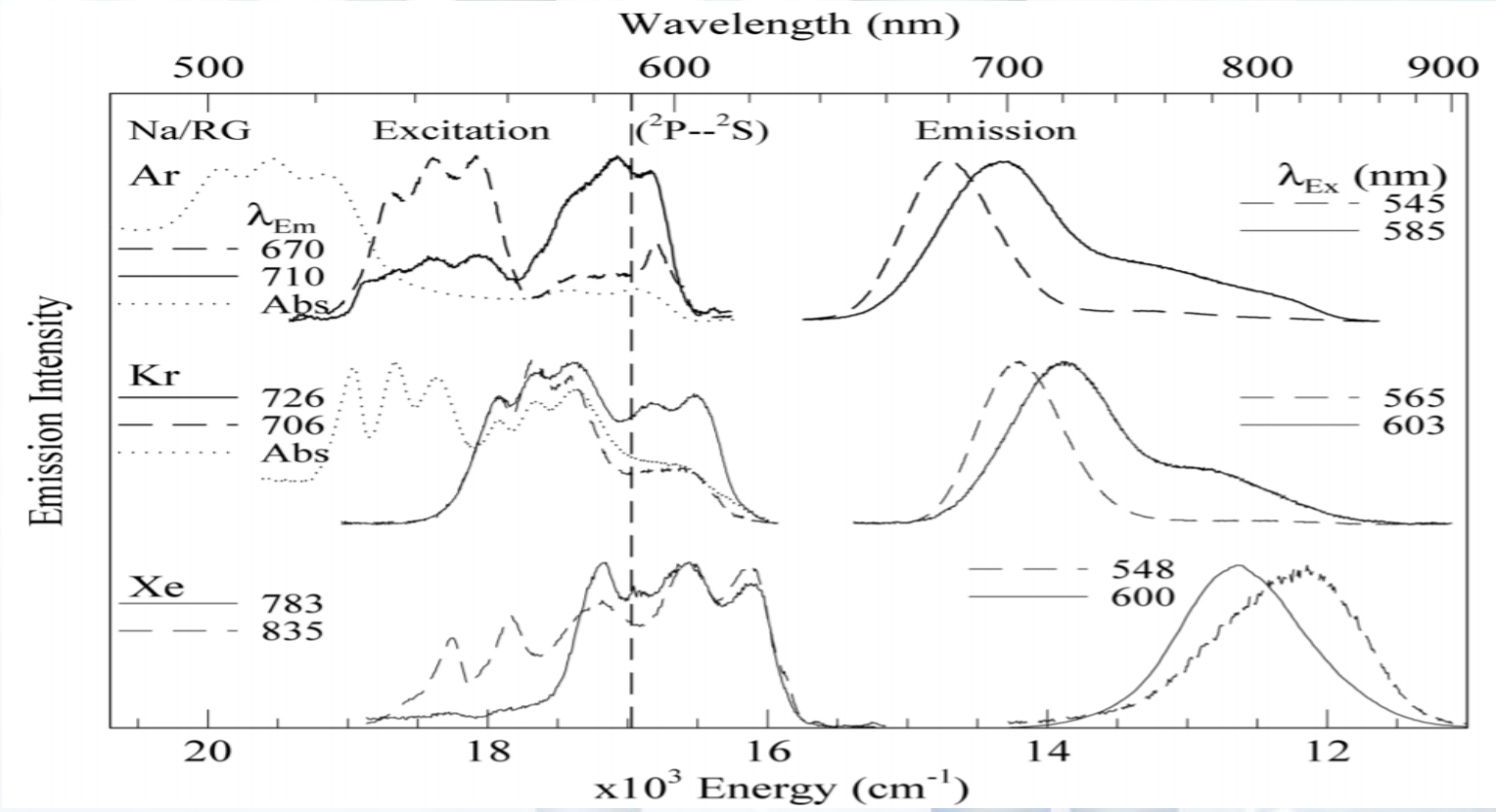


NIST Atomic Spectra Database Levels Data

$2p^6 3p$	$^2P^0$	1/2	16956,17025 $см^{-1}$
		3/2	16973,36619 $см^{-1}$

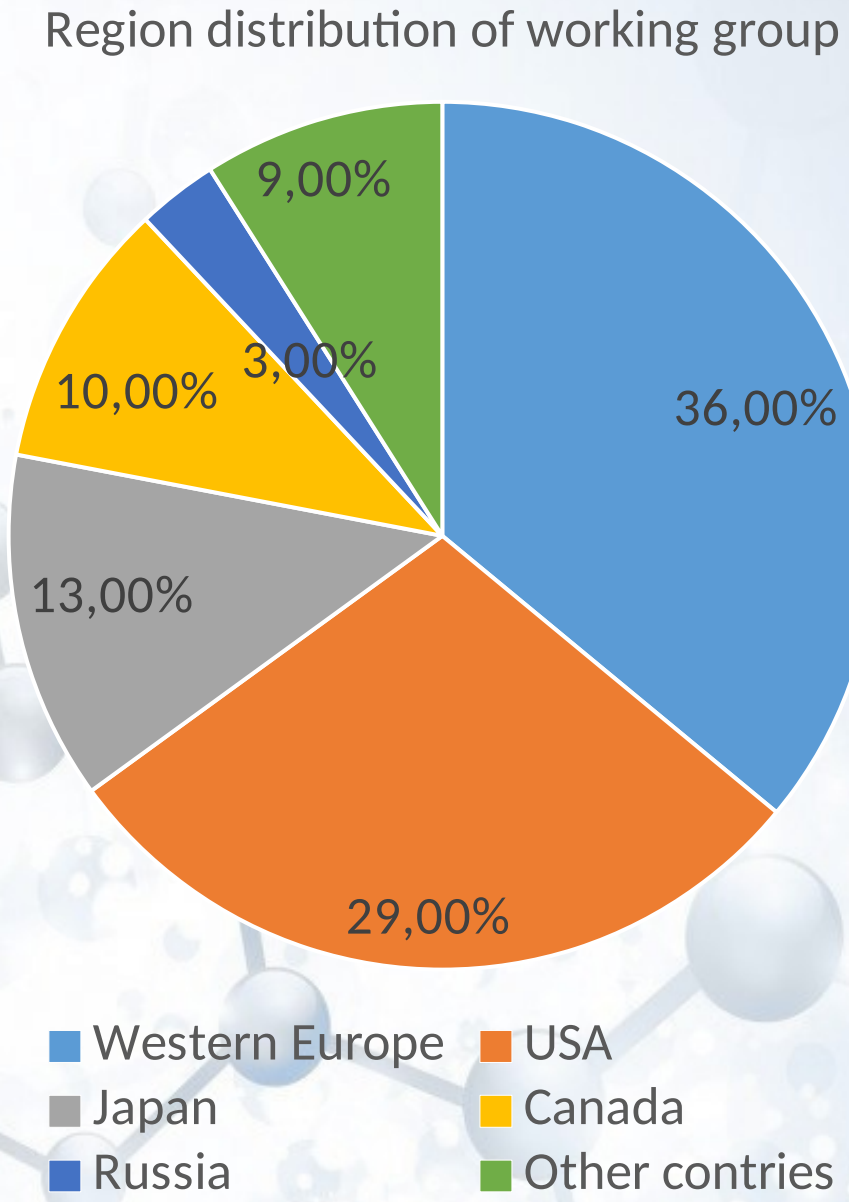
Матричная изоляция: проблемы (эксп)





Научное сообщество

~ 500 научных групп

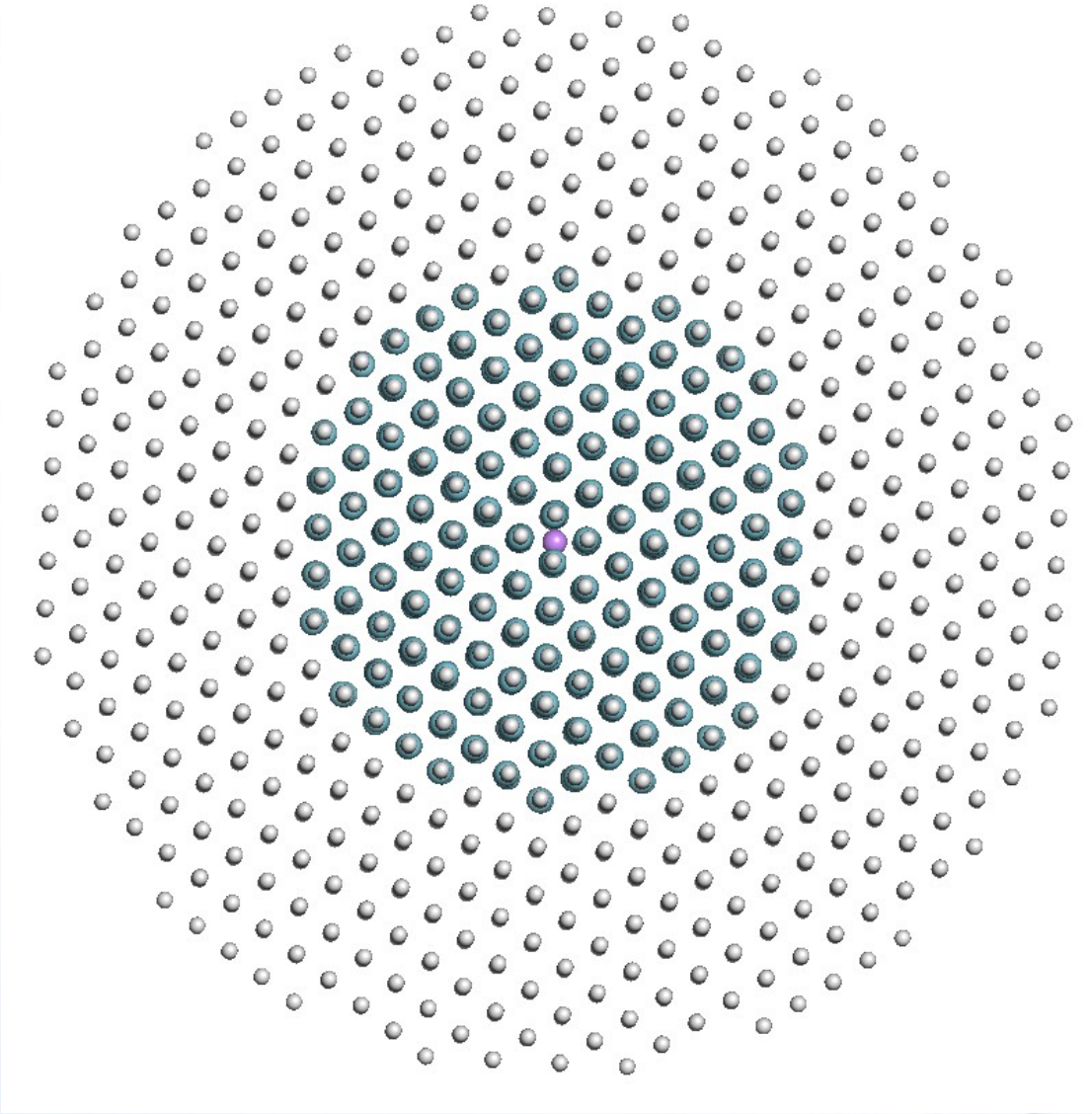


Основные конференции

The International Conferences on Low Temperature Chemistry and Physics

The International Conference on Cryocrystals and Quantum Crystals

Теоретическая модель



Подвижная область

Объем: 15 - 30 нм^3

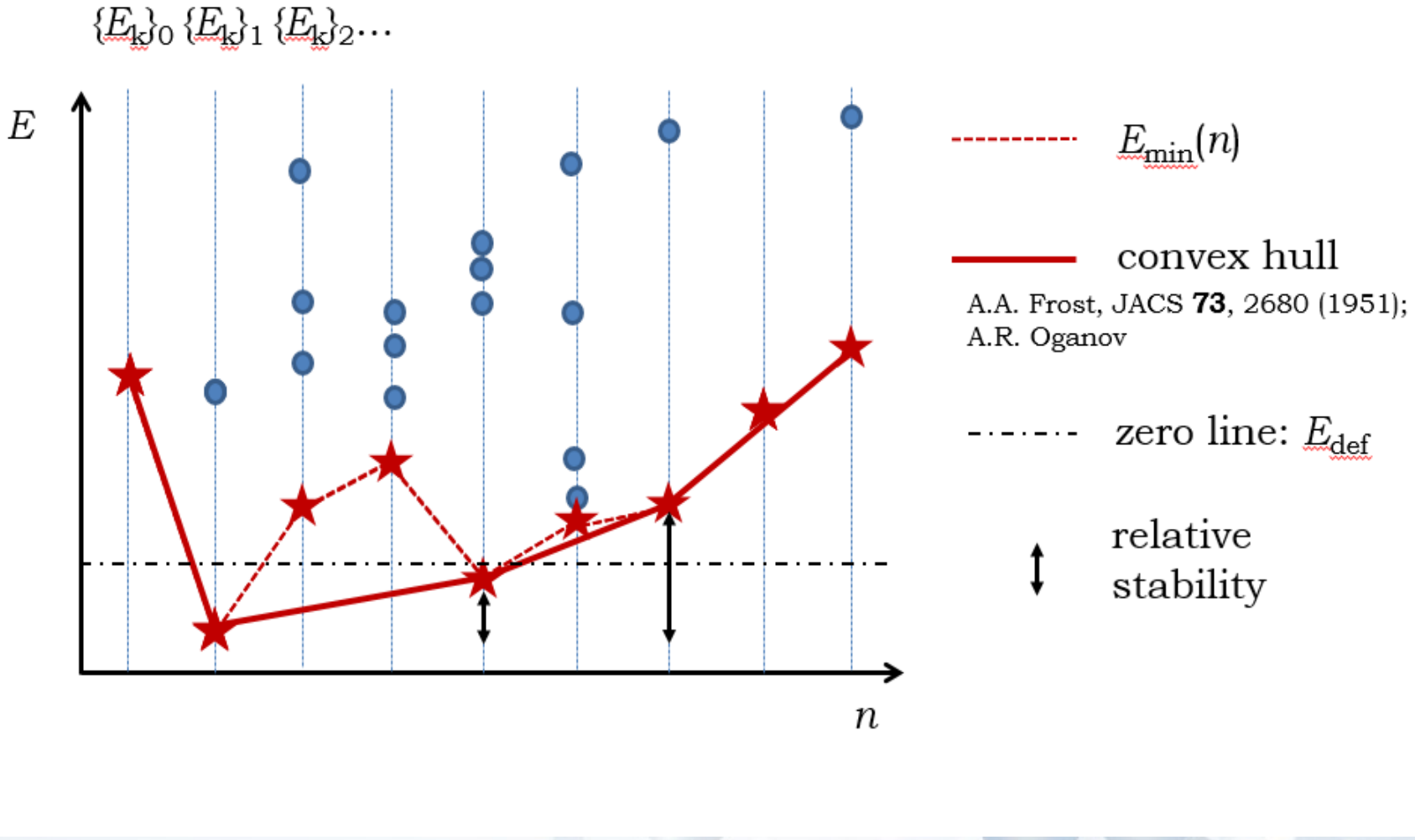
Атомов: 400 - 1000

Неподвижная область

Объем: 100 - 250 нм^3

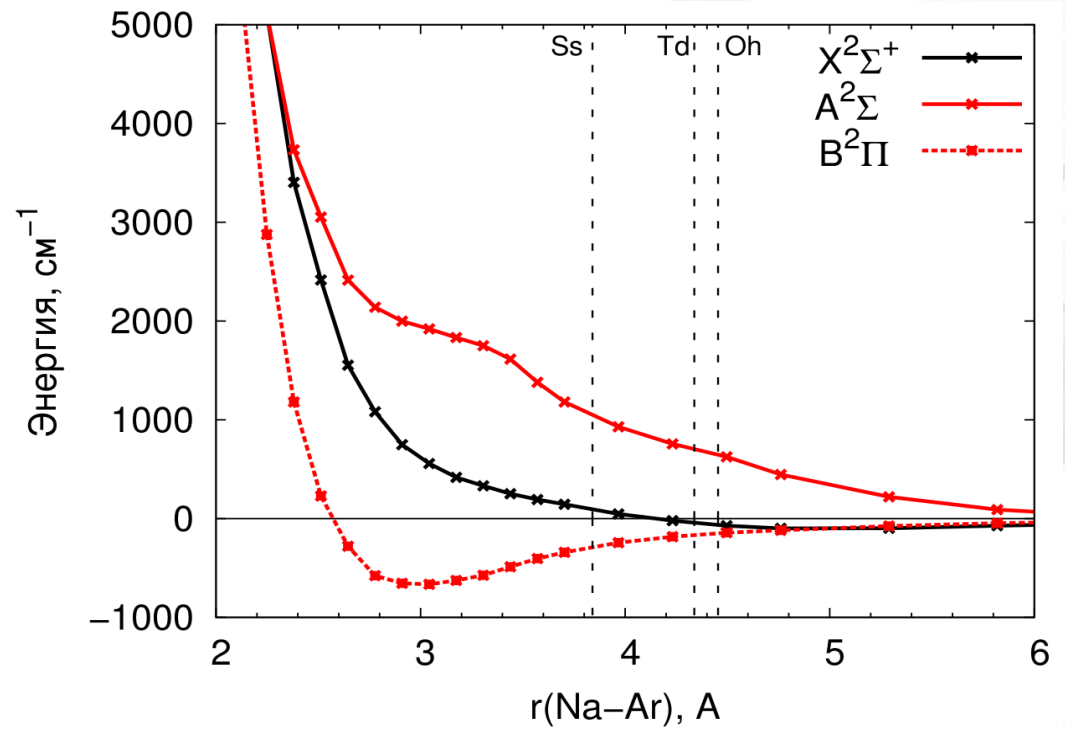
Атомов: 4000 - 10000

Метод выпуклой оболочки



Неэмпирические расчеты

MOLPRO



- CCSD(T) & CASSCF / MRCI (+Q)
- Связевые функции, CBS экстраполяция по серии Даннинга
- Stuggart RECP
- CO гамильтониан Брейта-Паули и поправки Дугласа-Кролла

- *DFT орбитали для CCSD(T), EOM-CCSD*

Молекулярная динамика

- Термодинамическое интегрирование проводится методом молекулярной динамики с термостатом Ланжевена

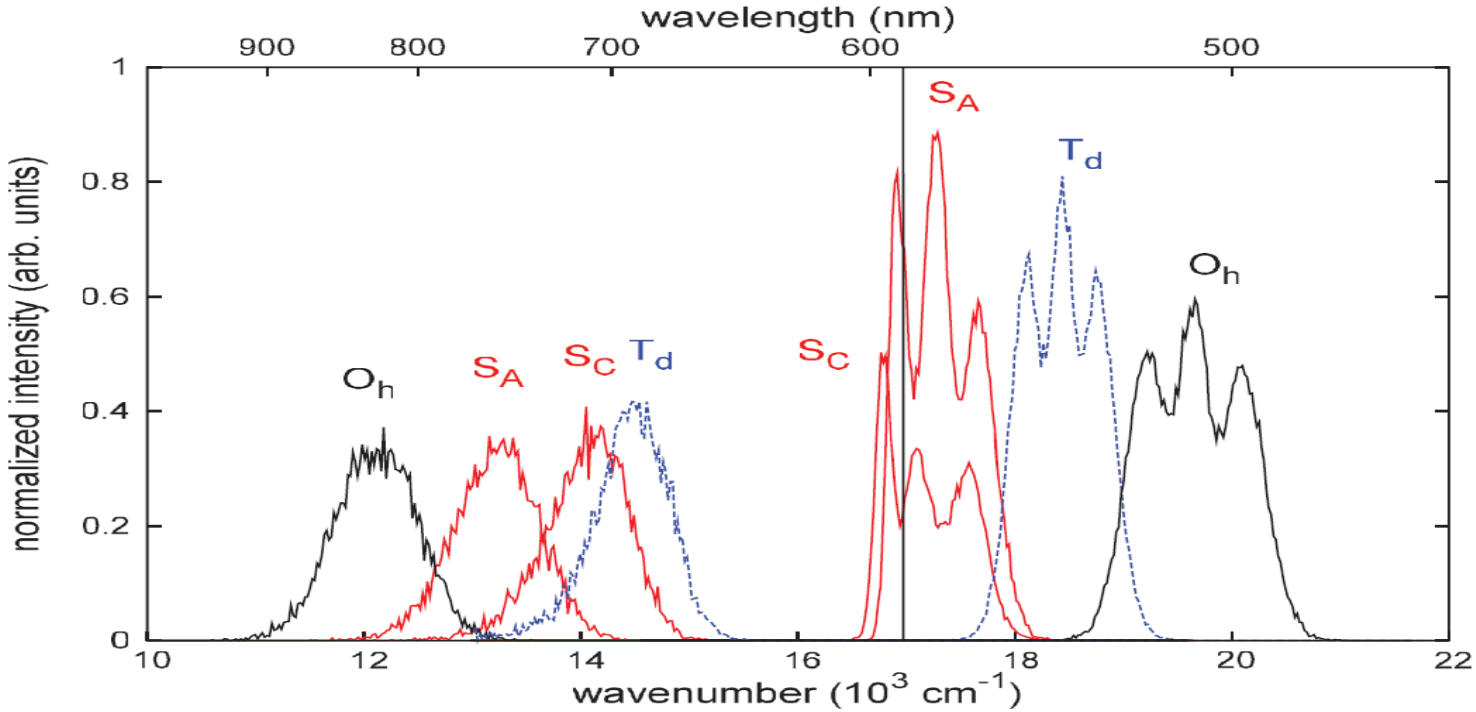
- Классическая температура МД моделирования корректируется в приближении Лакса (4K -> 25-40K)

$$T' = \frac{\hbar\omega}{2k_B}\left(\tanh\left(\frac{\hbar\omega}{2k_B T}\right)\right)^{-1}$$

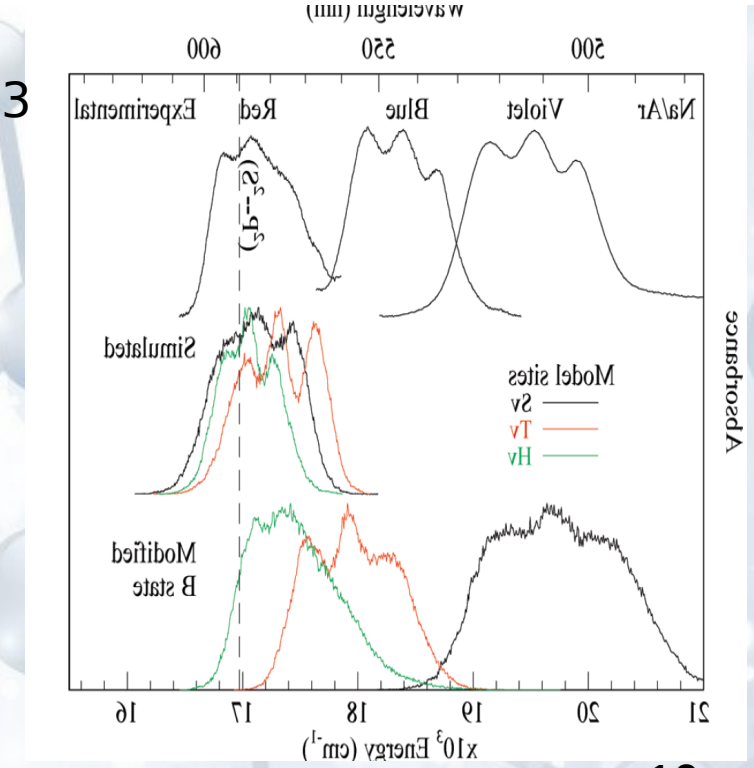
- Характерное время термолизации 50-200 пс

- Характерное время МД интегрирования 5-50 нс.

Na@Ar

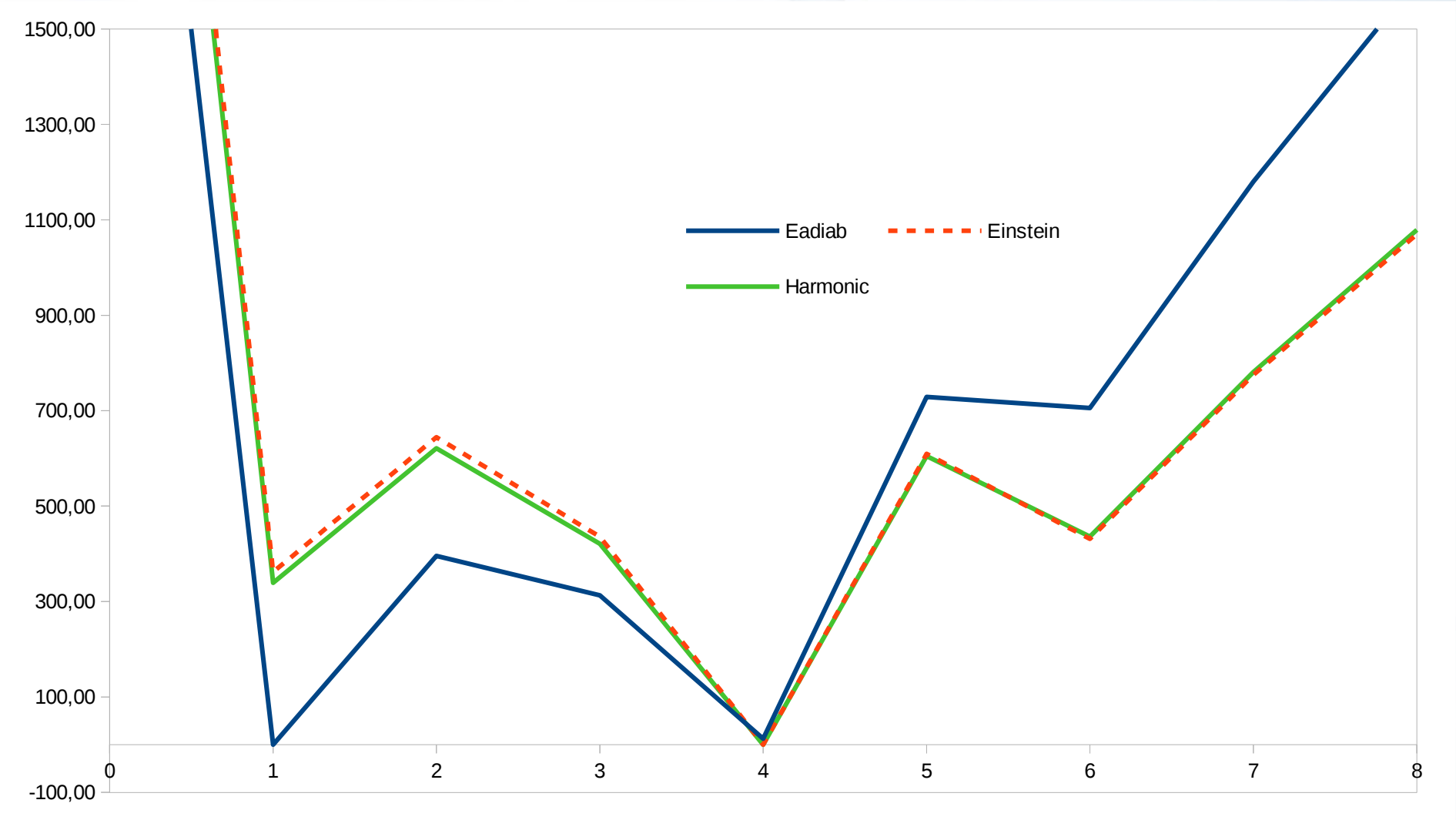


E. Jacquet et al // J. Chem. Phys. 135 (2011) 174503



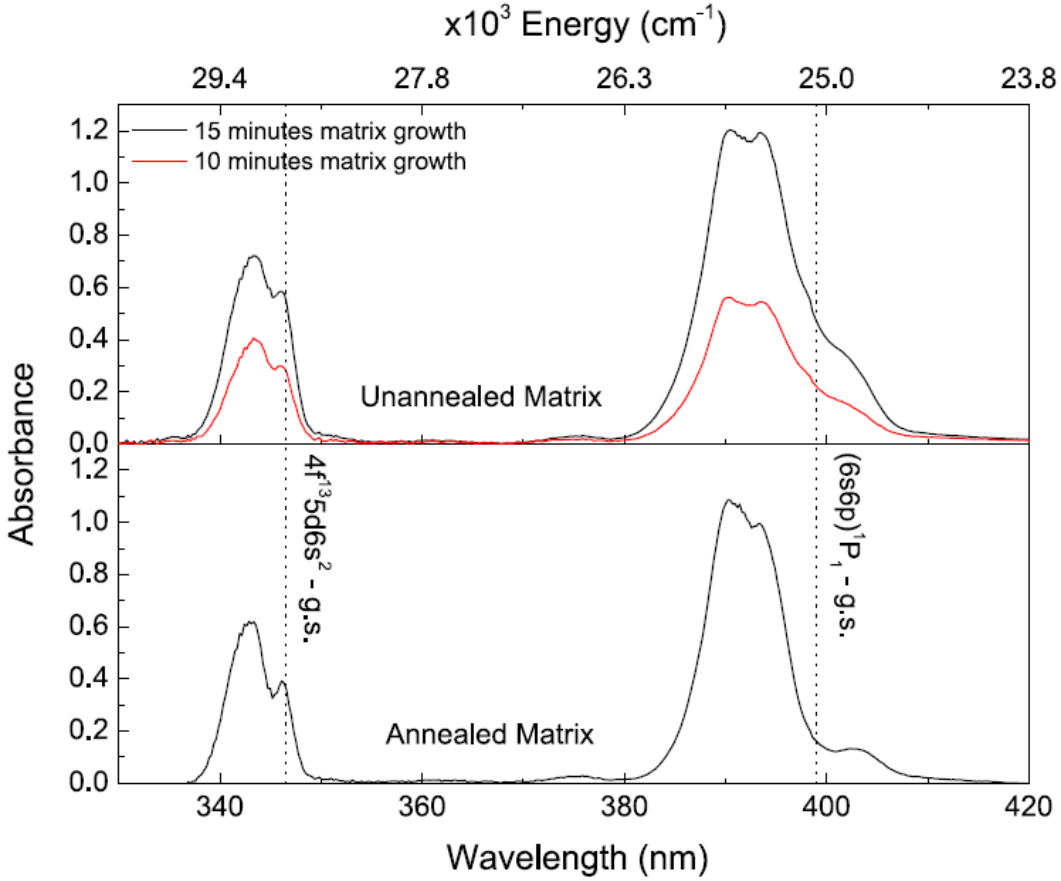
M. Ryan *et al*. // J. Phys. Chem. A 114 (2010) 3011

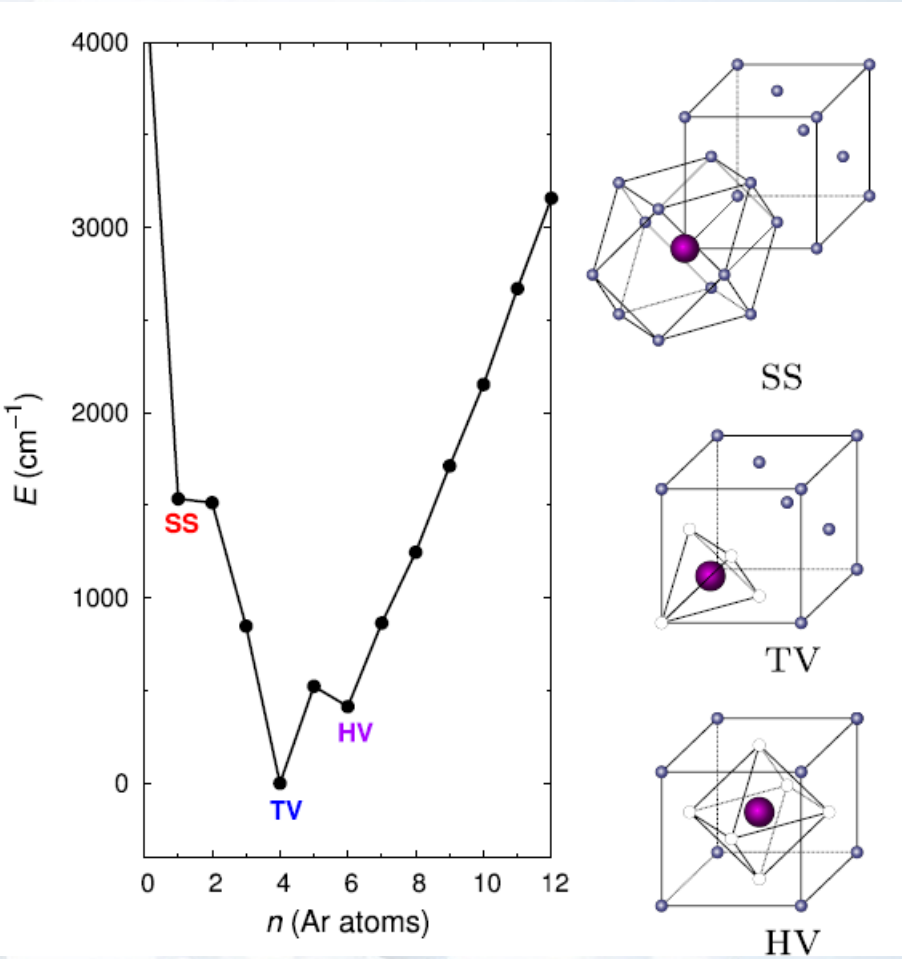
Na@Ar



A.V. Scherbinin, N.N. Kleshchina, D.S. Bezrukov, A.A. Buchachenko //PCCP (subm)

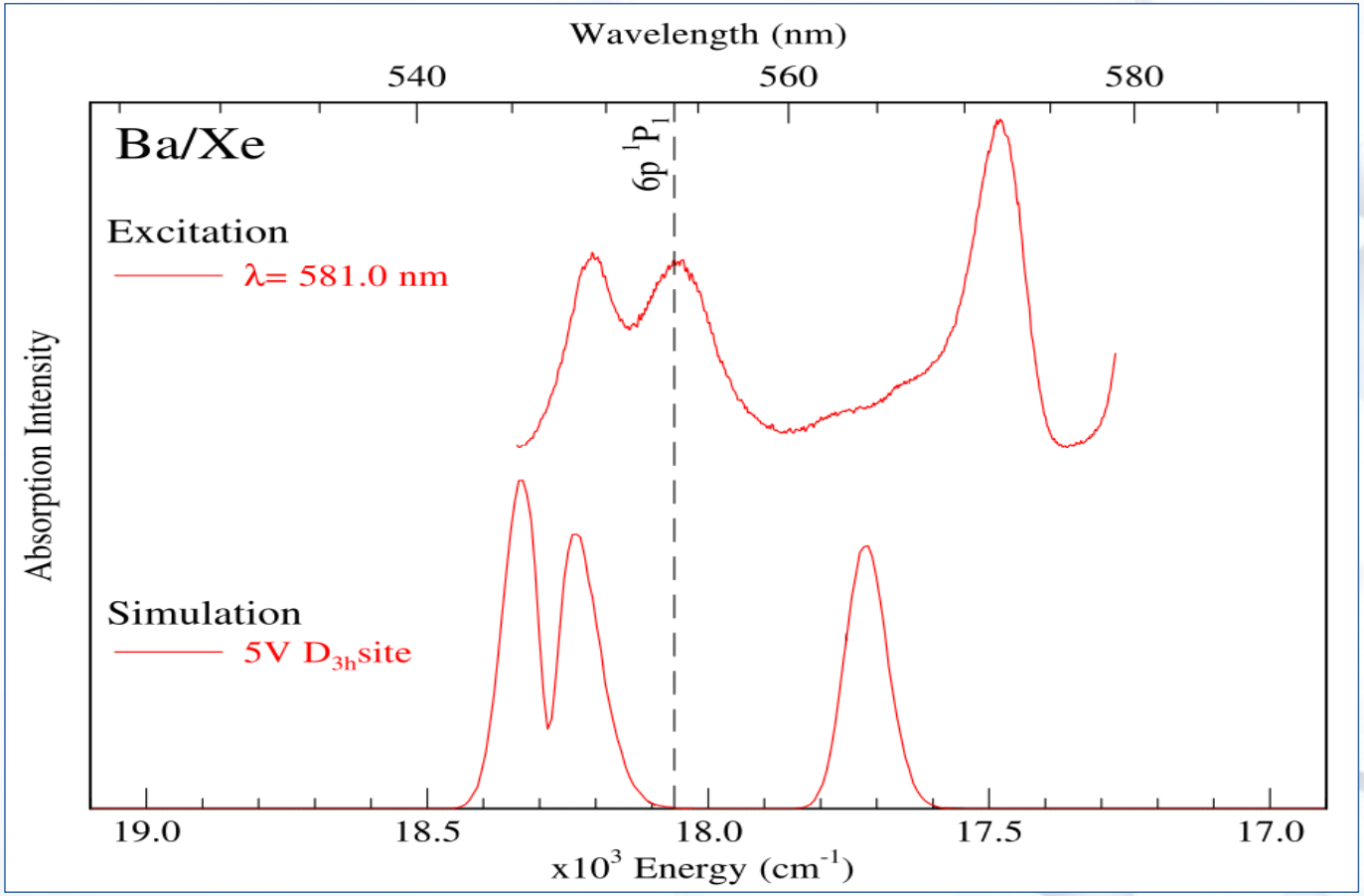
Yb@Ar

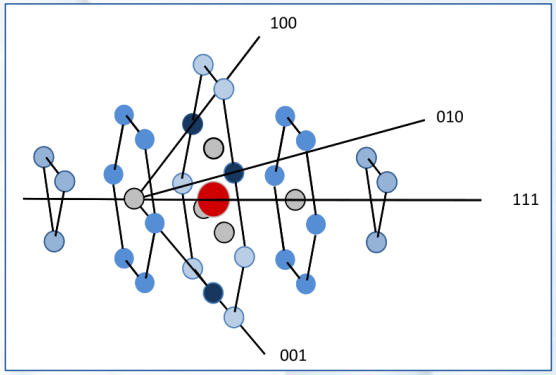




L.-G. Tao, N. N. Kleshchina, R. Lambo, A. A. Buchachenko, X.-G. Zhou, D. S. Bezrukov, S.-M. Hu. // J. Chem. Phys. 143 (2015) 174306

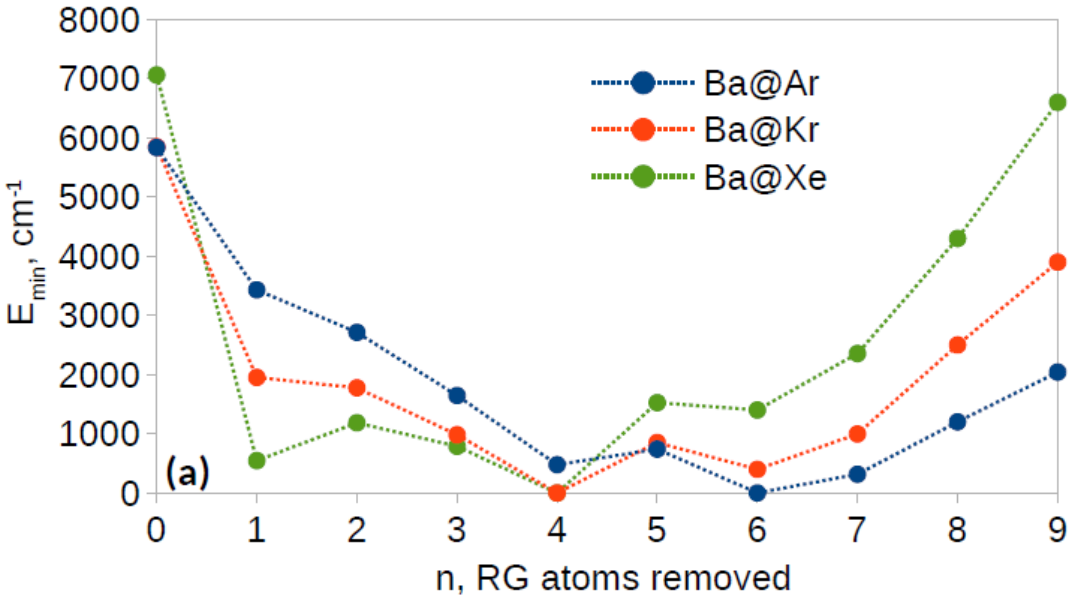
Ba@Xe

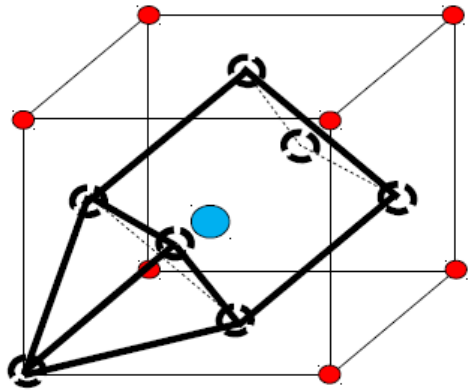




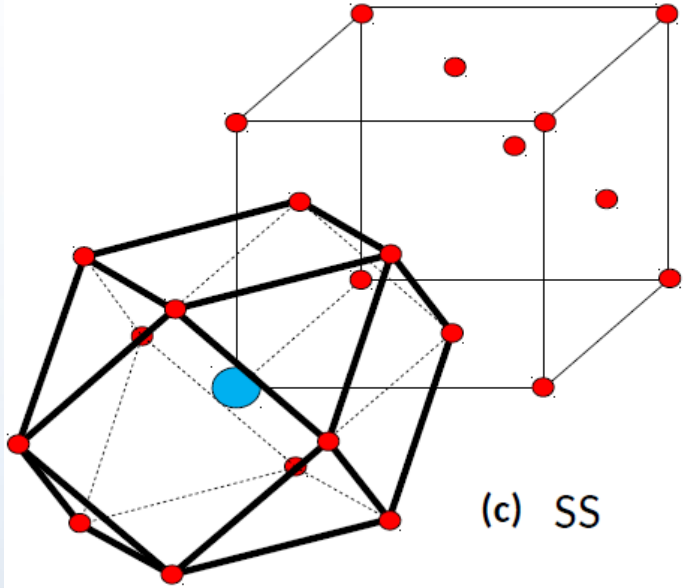
Davis B.M., Gervais B., McCaffrey J.G. // J. Chem. Phys. 148 (2018)24308.

Ba@Xe

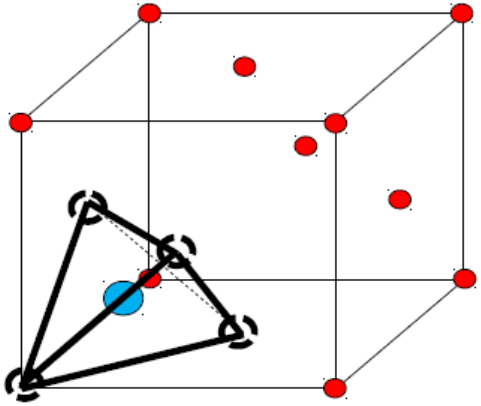




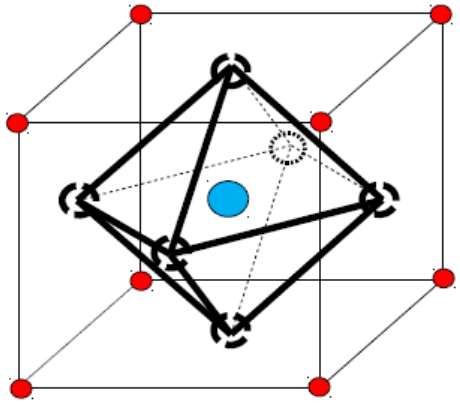
(b) S7



(c) SS



(d) TV



(e) HV

Ba@Xe


расчет
эксперимент
17200
17400
17600
17800
18000
18200
18400

Ван-дер-Ваальсовы димеры, Mn_2

Configuration	Term	*J*	Level (cm^{-1})
$3d^5 4s^2$	a ^6S	$^5/_2$	0.00
$3d^6(^5D)4s$	a ^6D	$^9/_2$	17 052.29
		$^7/_2$	17 282.00
		$^5/_2$	17 451.52
		$^3/_2$	17 568.48
		$^1/_2$	17 637.15

Ван-дер-Ваальсовы димеры, Mn_2

AIP | The Journal of Chemical Physics

Electronic structure and spin coupling of the manganese dimer: The state of the art of ab initio approach

Alexei A. Buchachenko, Grzegorz Chałasiński, and Małgorzata M. Szczęśniak

Citation: The Journal of Chemical Physics **132**, 024312 (2010); doi: 10.1063/1.3292572
View online: http://dx.doi.org/10.1063/1.3292572

State	R_e (Å)	D_e (cm^{-1})	D_0 (cm^{-1})	ω_e (cm^{-1})
$^1\Sigma^+_g$	3.605	572.6	551.4	42.4
$^3\Sigma^+_u$	3.615	568.8	547.7	42.3
$^5\Sigma^+_g$	3.633	561.9	540.8	42.0
$^7\Sigma^+_u$	3.653	552.3	531.2	41.5
$^9\Sigma^+_g$	3.674	540.5	519.3	41.0
$^{11}\Sigma^+_u$	3.691	534.0	512.4	41.4

Ван-дер-Ваальсовы димеры, Mn_2

THE JOURNAL OF PHYSICAL CHEMISTRY A

Article

pubs.acs.org/JPCA

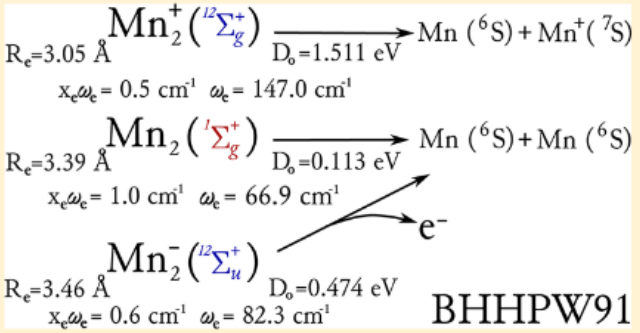
Neutral, Anionic, and Cationic Manganese Dimers through Density Functional Theory

Matteo Barborini*

S3 Research Center, CNR-NANO, Via Campi 213/a, 41125 Modena, Italy

Supporting Information

ABSTRACT: The manganese dimer is the only first row transition metal dimer that presents an antiferromagnetic $^1\Sigma_g^+$ ground state bonded by a van der Waals interaction. The various density functional theory (DFT) investigations devoted to the study of the ground state of this molecule and of its anionic and cationic states, are usually based on the generalized gradient approximation, giving results which contradict the experimental observations. In this work, we describe the overall spectroscopic properties of the neutral, cationic and anionic manganese dimers with DFT, focusing on understanding the effects of the percentage of Hartree−Fock exchange and of the different exchange-correlation functionals, on the relative stability of the various potential energy curves. For each of the three species we classify the ferromagnetic and antiferromagnetic states, studying the vertical detachment energies, the ionization energies and the electron affinities. In this way, we locate a hybrid exchange-correlation functional able to give for all the three species, results comparable with the experimental measurements and with previous accurate multiconfigurational calculations, defining a more accurate density functional theory approach to study larger charged or neutral manganese clusters.



Ван-дер-Ваальсовы димеры, Mn_2

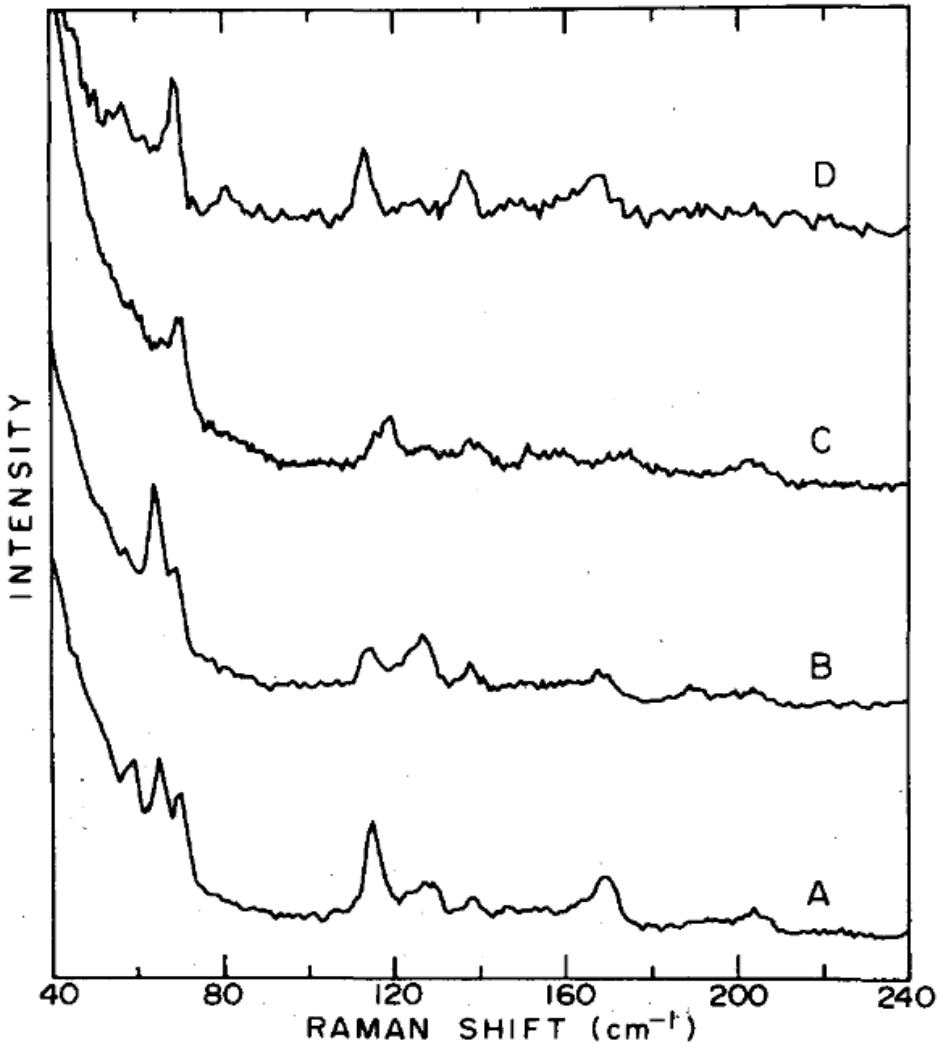
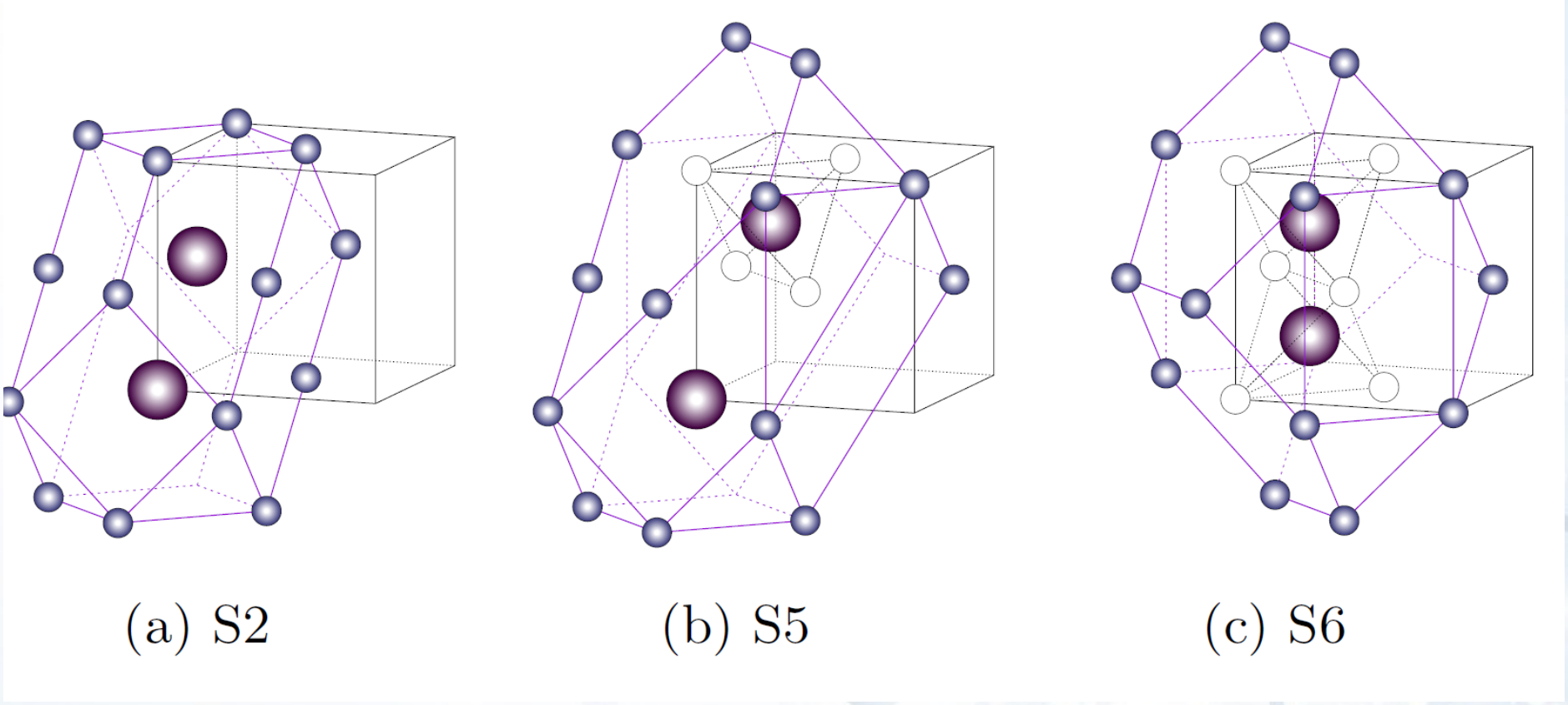


FIG. 7. Resonance Raman spectra of Mn_2 in solid Ar using 15 516 cm^{-1} dye laser radiation at (A) 13 K; (B) 13 K after prolonged exposure to laser irradiation; and (C) 23 K. (D) is the resonance Raman spectrum of Mn_2 in solid Ar using 14 840 cm^{-1} dye laser excitation.

K.D. Bier, T.L. Haslett, A.D. Kirkwood, M. Moskovits // J. Chem. Phys. 89 (1988) 6

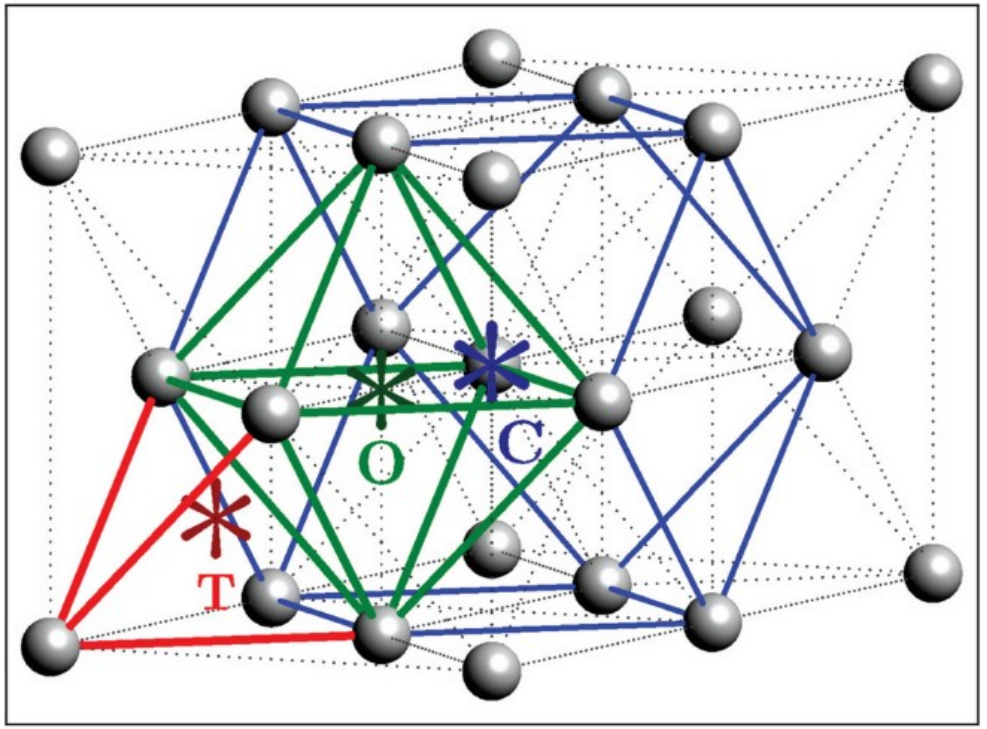
Ван-дер-Ваальсовы димеры, Mn_2



(a) S2 (b) S5 (c) S6

Общая карта ЛЖ кристаллов

Low Temperature Physics



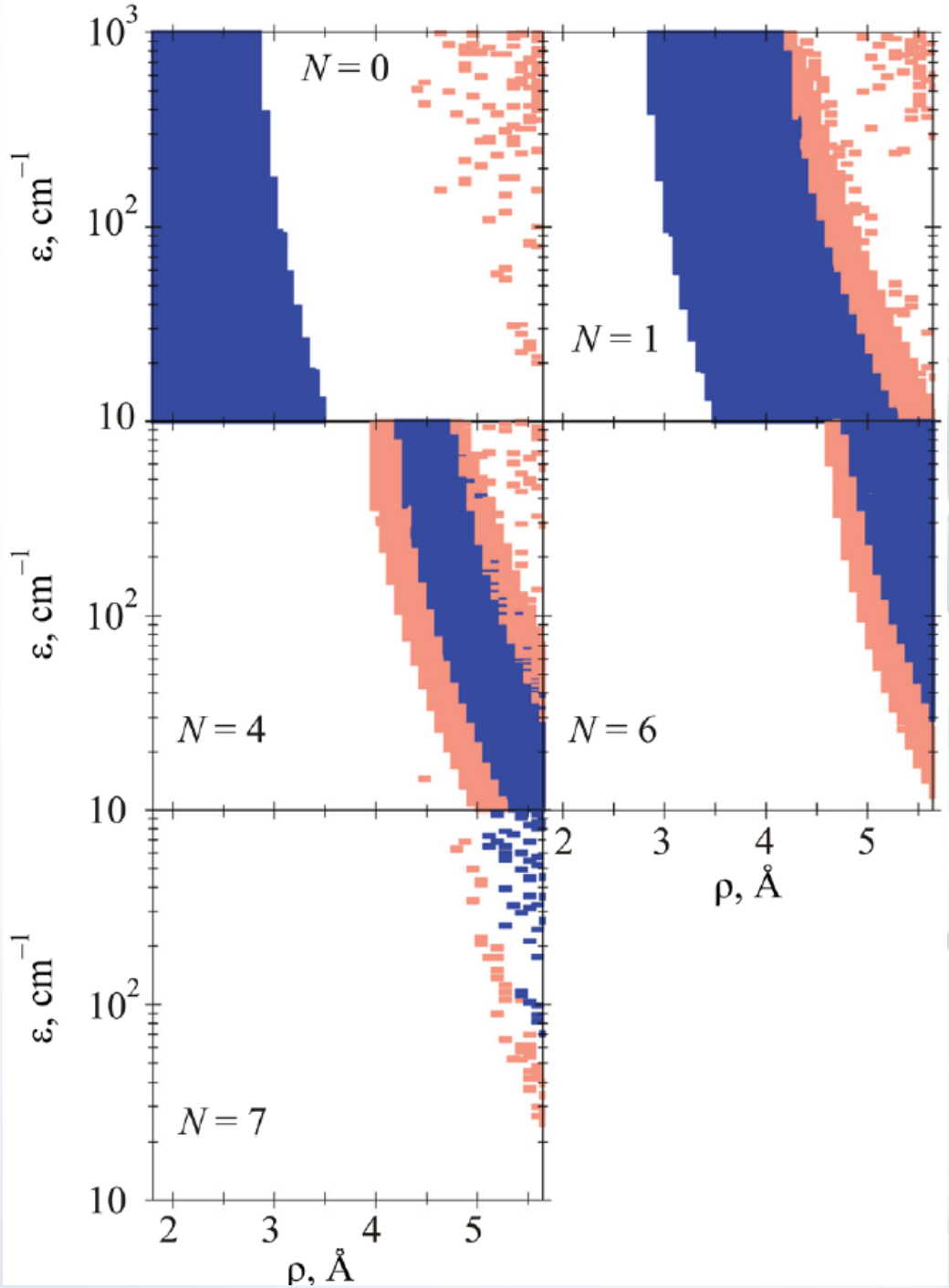
Volume 45, Issue 3, Mar. 2019

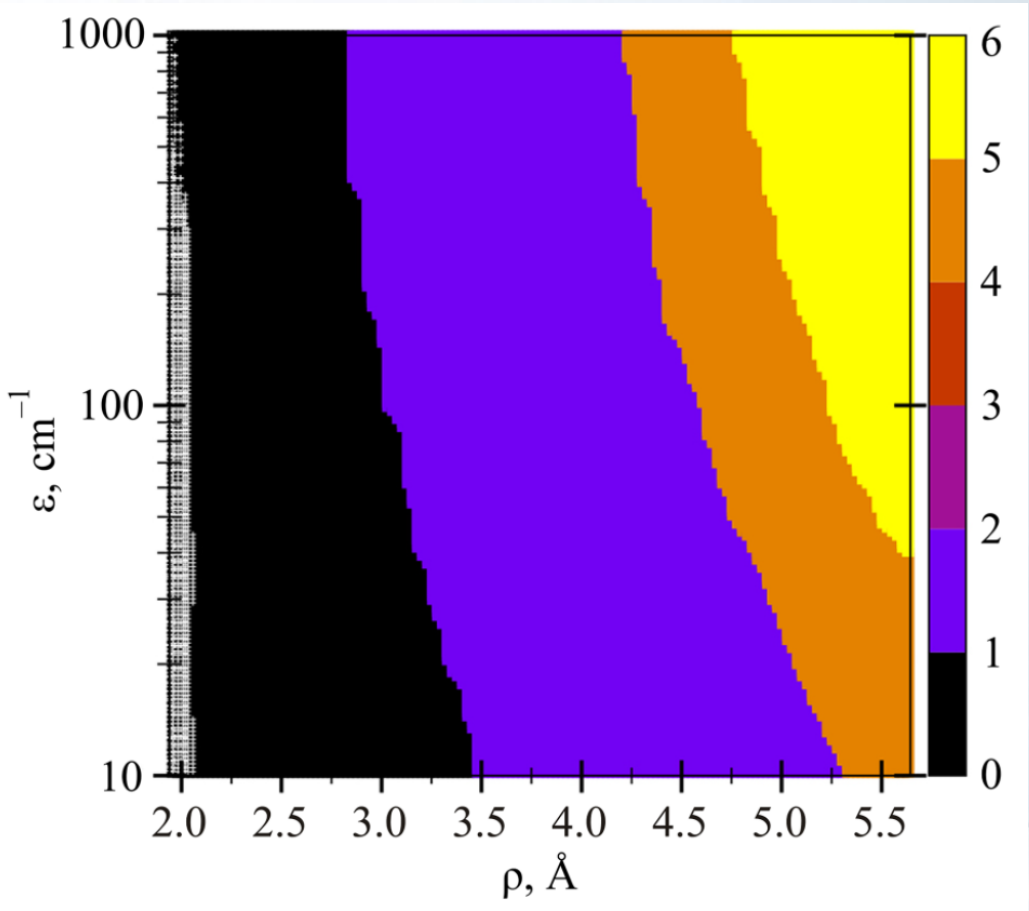
Computational study of the stable atomic trapping sites in Ar lattice

Low Temp. Phys. **45,** 301 (2019); doi.org/10.1063/1.5090045

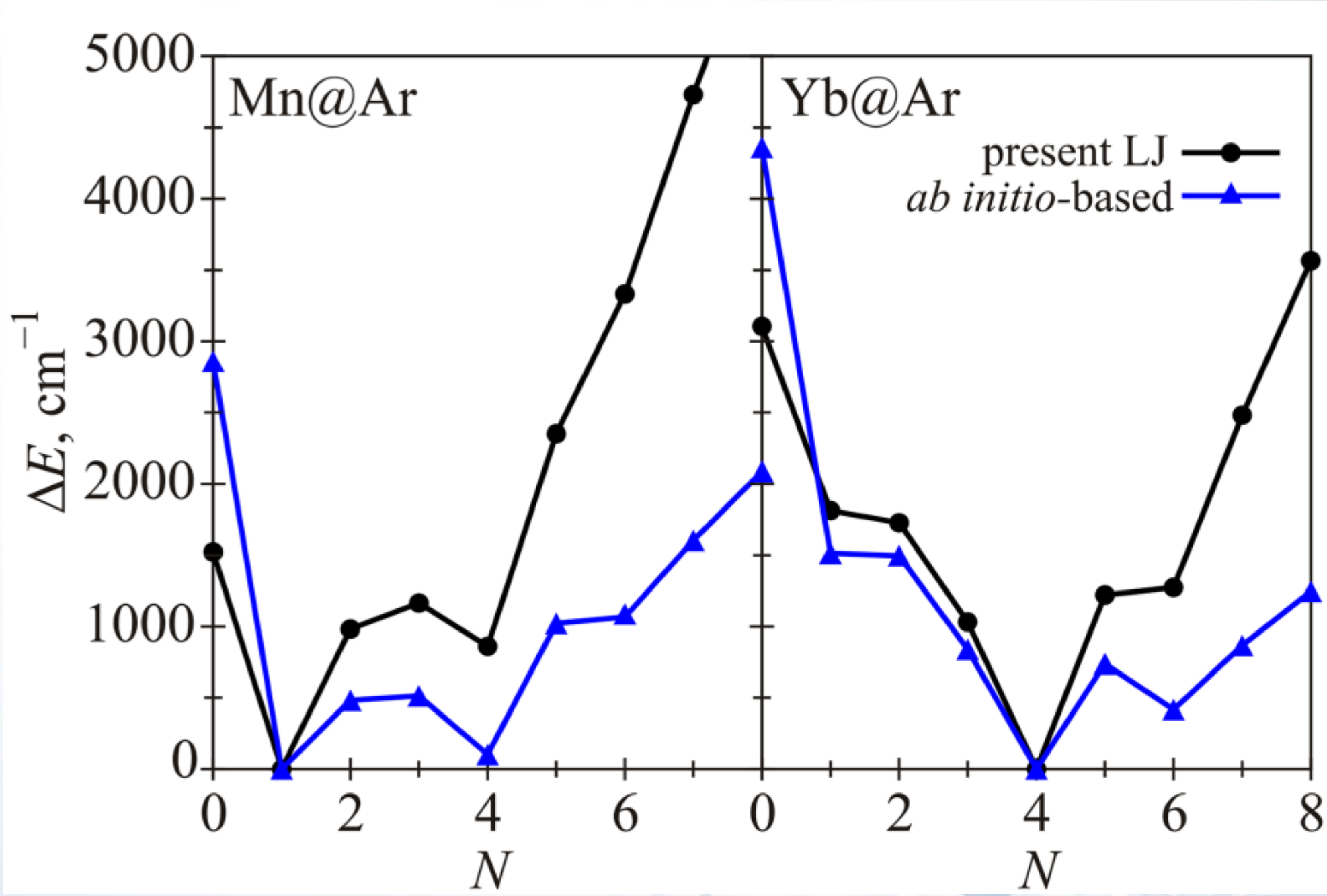
G. K. Ozerov, D. S. Bezrukov, and A. A. Buchachenko

Общая карта ЛЖ кристаллов





Общая карта ЛЖ кристаллов



Текущие задачи

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Enriched Xenon Observatory

From Wikipedia, the free encyclopedia

Coordinates: 32°22′18″N 103°47′37″W

The **Enriched Xenon Observatory (EXO)** is a particle physics experiment searching for neutrinoless double beta decay of xenon-136 at WIPP near Carlsbad, New Mexico, U.S.

Neutrinoless double beta decay (0νββ) detection would prove the Majorana nature of neutrinos and impact the neutrino mass values and ordering. These are important open topics in particle physics.

EXO currently has a 200-kilogram xenon liquid time projection chamber (**EXO-200**) with R&D efforts on a ton-scale experiment (**nEXO**). Xenon double beta decay was detected and limits have been set for 0νββ.

- Схема двойного безнейтринного бета-распада:

$$Xe \longrightarrow Ba^{2+} + 2e^{-}$$

- Ba^{2+} частично нейтрализуется окружением

$$Ba^{2+} + Xe_{liq} \longrightarrow Ba^{+} + Xe_{liq}(e^{-})$$

- Отбор криопроб и анализ на наличие Ba^{+}

Текущие задачи

PHYSICAL REVIEW A **91**, 022505 (2015)

Spectroscopy of Ba and Ba^+ deposits in solid xenon for barium tagging in nEXO

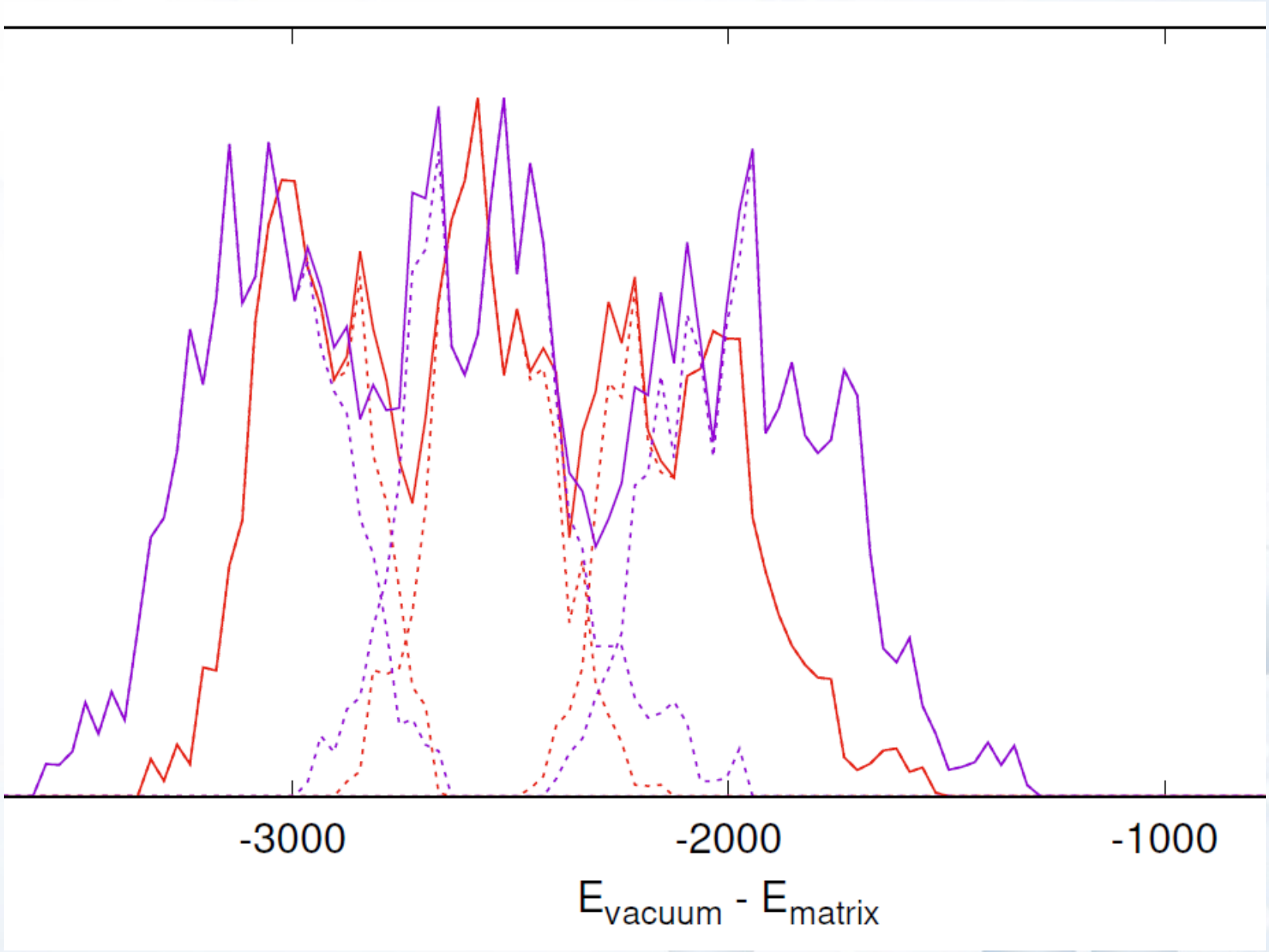
B. Mong,[1,2] S. Cook,[1,*] T. Walton,[1] C. Chambers,[1] A. Craycraft,[1] C. Benitez-Medina,[1,†] K. Hall,[1,‡] W. Fairbank, Jr.,[1,§] J. B. Albert,[3] D. J. Auty,[4] P. S. Barbeau,[5] V. Basque,[6] D. Beck,[7] M. Breidenbach,[8] T. Brunner,[9] G. F. Cao,[10] B. Cleveland,[2,‖] M. Coon,[7] T. Daniels,[8] S. J. Daugherty,[3] R. DeVoe,[9] T. Didberidze,[4] J. Dilling,[11] M. J. Dolinski,[12] M. Dunford,[6] L. Fabris,[13] J. Farine,[2] W. Feldmeier,[14] P. Fierlinger,[14] D. Fudenberg,[9] G. Giroux,[15,¶] R. Gornea,[15] K. Graham,[6] G. Gratta,[9] M. Heffner,[16] M. Hughes,[4] X. S. Jiang,[10] T. N. Johnson,[3] S. Johnston,[17] A. Karelin,[18] L. J. Kaufman,[3] R. Killick,[6] T. Koffas,[6] S. Kravitz,[9] R. Krücken,[11] A. Kuchenkov,[18] K. S. Kumar,[19] D. S. Leonard,[20] C. Licciardi,[6] Y. H. Lin,[12] J. Ling,[7] R. MacLellan,[21] M. G. Marino,[14] D. Moore,[9] A. Odian,[8] I. Ostrovskiy,[9] A. Piepke,[4] A. Pocar,[17] F. Retiere,[11] P. C. Rowson,[8] M. P. Rozo,[6] A. Schubert,[9] D. Sinclair,[6,11] E. Smith,[12] V. Stekhanov,[18] M. Tarka,[7] T. Tolba,[15] K. Twelker,[9] J.-L. Vuilleumier,[15] J. Walton,[7] M. Weber,[9] L. J. Wen,[10] U. Wichoski,[2] L. Yang,[7] Y.-R. Yen,[12] and Y. B. Zhao[10]
(nEXO Collaboration)

Absorption spectroscopy of heavy alkaline earth metals Ba and Sr in rare gas matrices —CCSD(T) calculations and atomic site occupancies

Cite as: J. Chem. Phys. **144**, 044308 (2016); https://doi.org/10.1063/1.4940688
Submitted: 02 November 2015 . Accepted: 08 January 2016 . Published Online: 29 January 2016

Barry M. Davis, and John G. McCaffrey

Текущие задачи



Текущие задачи

atoms

MDPI

Article

Oriented Polar Molecules in a Solid Inert-Gas Matrix: A Proposed Method for Measuring the Electric Dipole Moment of the Electron

A. C. Vutha [1,*], M. Horbatsch [2] and E. A. Hessels [2]

[1] Department of Physics, University of Toronto, Toronto, ON, M5S 1A7, Canada
[2] Department of Physics and Astronomy, York University, Toronto, ON, M3J 1P3, Canada; marko@yorku.ca (M.H.); hessels@yorku.ca (E.A.H.)
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Received: 24 October 2017; Accepted: 27 December 2017; Published: 5 January 2018

Ключевые пункты доклада

Матричная изоляция преставляет интерес для достаточно небольшой части нучного сообщества, при этом задачи весьма разнородны – от описания стабильных сайтов захвата до описания кинетических систем

Предложен, разработан и успешно апробирован метод определения стабильных сайтов захвата в матрицах инертных газов

Впервые описаны в литературе сайты захвата вида 7V для S атомов и сайты 5V для димеров

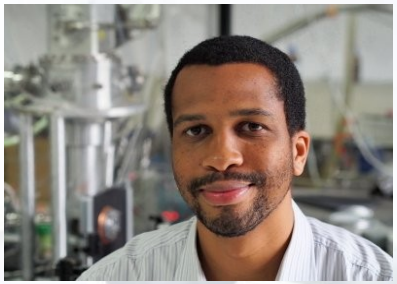
При помощи проведения достаточно больших вычислительных экспериментов выдвинуто предположение об отсутствии в случае S атомов стабильных сайтов 2V, 3V и 5V

Интересных задач много, работа продолжается!

Коллеги и поддержка

Skolkovo Tech
Skolkovo Institute of Science and Technology

MSU



Dr Ricardo Lewis Lambo
Physical Chemistry Dep.
University of Science and Technology of China
Hefei National Lab. For Phys. Sciences at the Microscale

Maynooth University
National University of Ireland Maynooth

Dr John G. McCaffrey
National University of Ireland Maynooth
Department of Chemistry

Georgiy Ozerov, **Alexei Buchachenko**,
Victor Vysotsky, Nadya Kleshchina,
Inga Kalinina, **Dmitriy Bezrukov**,
Andrey Scherbinin, Boris Kamorzin

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