Acceleration of chemical reactions in hybrid one-dimensional photonic crystals based on high-index metamaterials

A. I. Garifullin[1], R. Kh. Gainutdinov[1,2], M. A. Khamadeev[1,2]

[1]Institute of Physics, Kazan Federal University, Kazan, 420008 Russia
[2]Institute of Applied Research, Tatarstan Academy of Sciences, Kazan, 420111 Russia

e-mail: adel-garifullin@mail.ru

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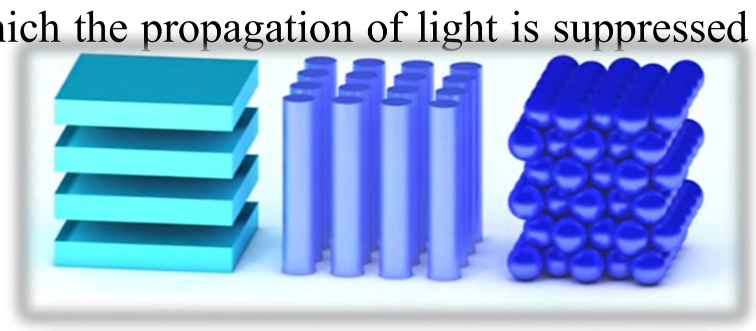
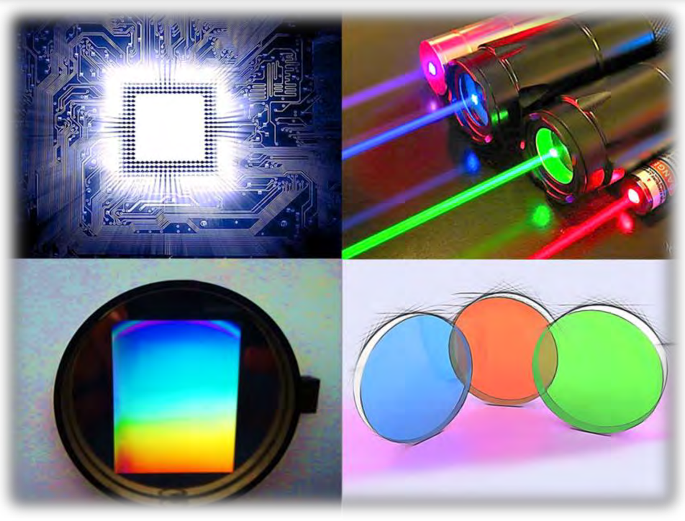
New artificial media like photonic crystals and metamaterials

Photonic Crystals (PCs) are artificial media, where refractive index varies periodically in space with a period comparable to the optical wavelength range [1].

Photonic Bandgaps are the spectral ranges of a PC for which the propagation of light is suppressed due to the diffraction by a periodic structure of PCs.



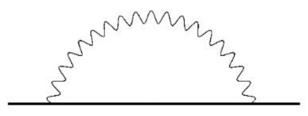


Application of PCs and metamaterials:

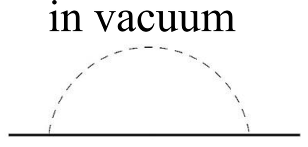
- High-quality resonators, lasers, interference filters,
- Diffractional lattice, waveguides, polarizers
- Sensors
- Epsilon-near zero, negative refractive index, highly tunable refractive index materials

Quantum electrodynamic (QED) effects in PCs:

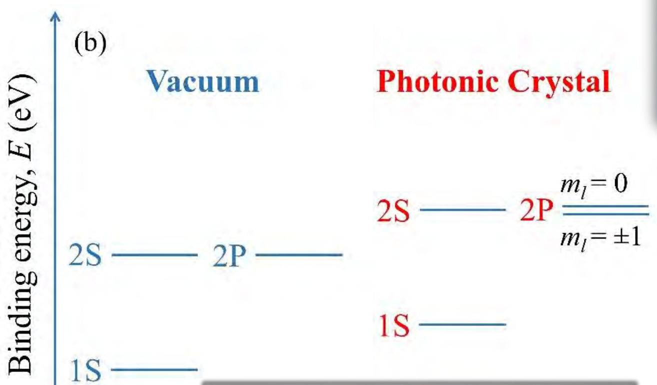
- Control of spontaneous emission
- Photon-atom bound state
- ***Change of an electromagnetic mass of an electron [2]***

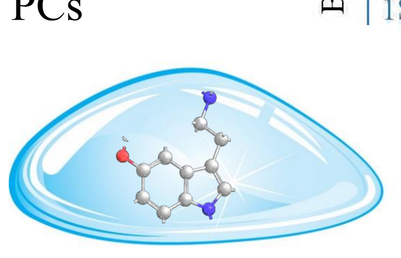


Atomic electron in vacuum

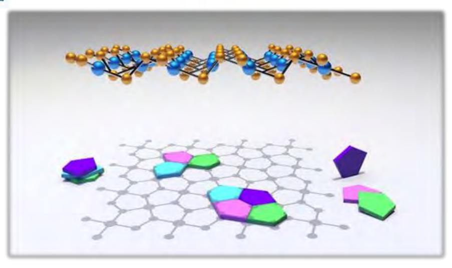


Atomic electron in PCs

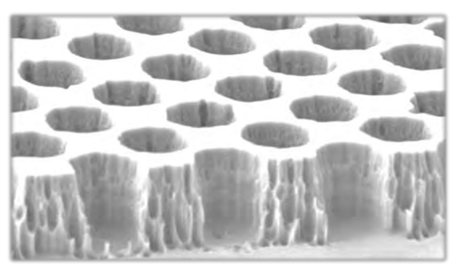




Microdroplets chemistry



Synthesis of new chemical compounds and drugs



Chemical reactions in nanoporous materials

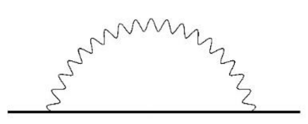
Nowadays one of the most important physicochemical problems is acceleration of chemical and biochemical reactions in confined environment (microdroplets, colloidal nanocrystal assemblies, *etc.*)

The aim of this work:

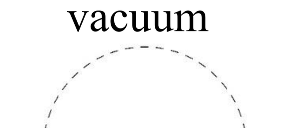
Development of the experimental verification method of the electron electromagnetic mass change effect based on the observation of shifts in the spectral lines of helium atoms injected in the gas phase in air voids of a hybrid one-dimensional photonic crystal by optical spectroscopy techniques.

The self-energy correction to the electromagnetic mass of an electron in PCs

$\hbar = c = 1$



Free electron in vacuum

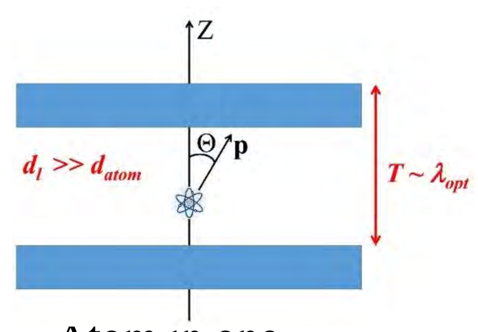


Free electron in PCs

$$m_e = m_0 + m_{em}$$

$$m_e^{pc} = m_0 + m_{em}^{pc}$$

$$\delta m_{pc} = m_{em}^{pc} - m_{em}$$



Atom in one-dimensional PC

$$E + \Delta E_{em}^{pc}(\hat{\mathbf{p}}) = \left(m_e + \delta m_{pc}(\hat{\mathbf{I}}_{\mathbf{p}})\right)c^2 + \frac{\hat{\mathbf{p}}^2}{2\left(m_e + \delta m_{pc}(\hat{\mathbf{I}}_{\mathbf{p}})\right)},$$

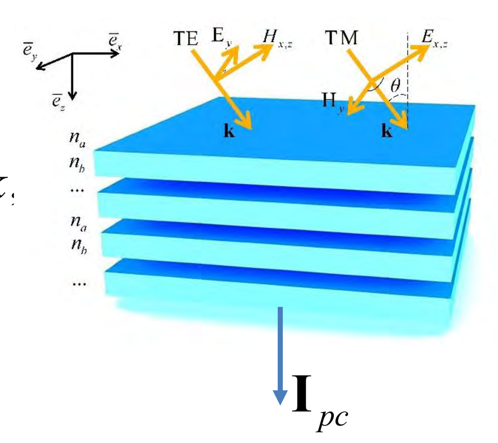
$\hat{\mathbf{I}}_{\mathbf{p}}$ is the operator of the electron momentum direction

$$\delta m_{pc}(\hat{\mathbf{I}}_{\mathbf{p}}) = A + \left(\hat{\mathbf{I}}_{\mathbf{p}} \cdot \hat{\mathbf{I}}_{pc}\right)^2 B,$$

where

$$A = \frac{\alpha}{\pi}\sum_{n,G}\int k_\rho dk_\rho \int_{FBZ} dk_z \left(\frac{|E_{\mathbf{k}n1}(G)|^2}{\omega_{\mathbf{k}n1}^2}\frac{k_{Gz}^2}{k_\rho^2 + k_{Gz}^2} + \frac{|E_{\mathbf{k}n2}(G)|^2}{\omega_{\mathbf{k}n2}^2}\right) - \frac{4\alpha}{3\pi}\int dk,$$

$$B = \frac{\alpha}{\pi}\sum_{n,G}\int k_\rho dk_\rho \int_{FBZ} dk_z \left(\frac{|E_{\mathbf{k}n1}(G)|^2}{\omega_{\mathbf{k}n1}^2}\frac{2k_\rho^2 - k_{Gz}^2}{k_\rho^2 + k_{Gz}^2} - \frac{|E_{\mathbf{k}n2}(G)|^2}{\omega_{\mathbf{k}n2}^2}\right),$$



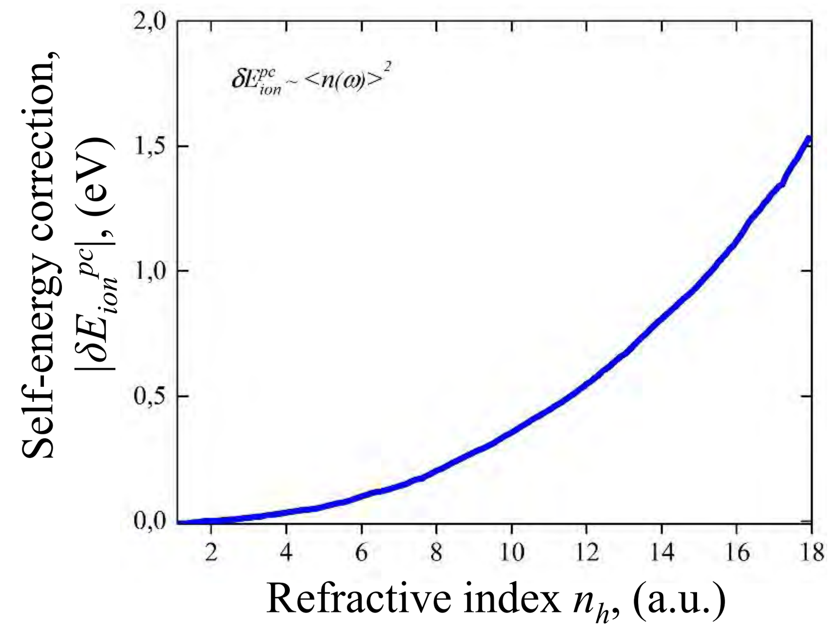
Z-axis of 1D PC

where $\omega_{\mathbf{k}n1}, \omega_{\mathbf{k}n2}$ are the dispersion relations for TE (transverse electric) and TM (transverse magnetic) electromagnetic field [3].

This is the PC correction to the free electron electromagnetic mass. The charged particle is placed in an air void of a 1D PC, thus, this correction is derived with using cylindrical symmetry. For the case of an atomic electron, it is necessary to calculate the matrix elements with using the electron wavevectors in appropriate electron states.

The self-energy correction to the ionization energy of atoms in 1D PCs

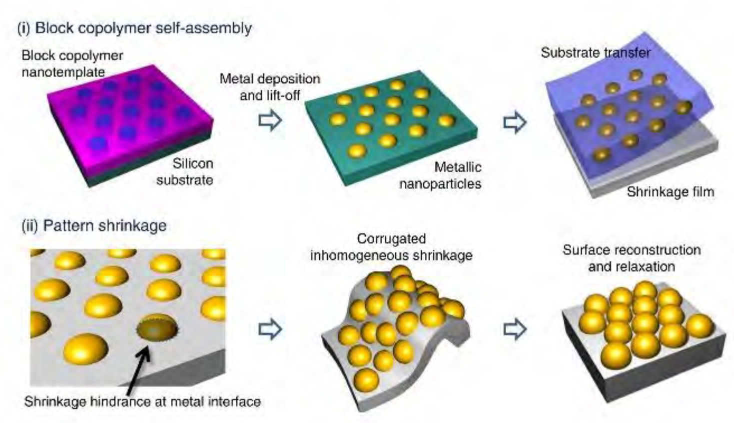
$$\delta E_{ion}^{pc} = -\frac{2\alpha}{3\pi}\sum_{n,G}\left[\int k_\rho dk_\rho \int_{FBZ} dk_z \left(\frac{|E_{\mathbf{k}n1}(G)|^2}{\omega_{\mathbf{k}n1}^2}\cdot\frac{k_{Gz}^2 - 2k_\rho^2}{k_\rho^2 + k_{Gz}^2} + \frac{|E_{\mathbf{k}n2}(G)|^2}{\omega_{\mathbf{k}n2}^2}\right)\right],$$



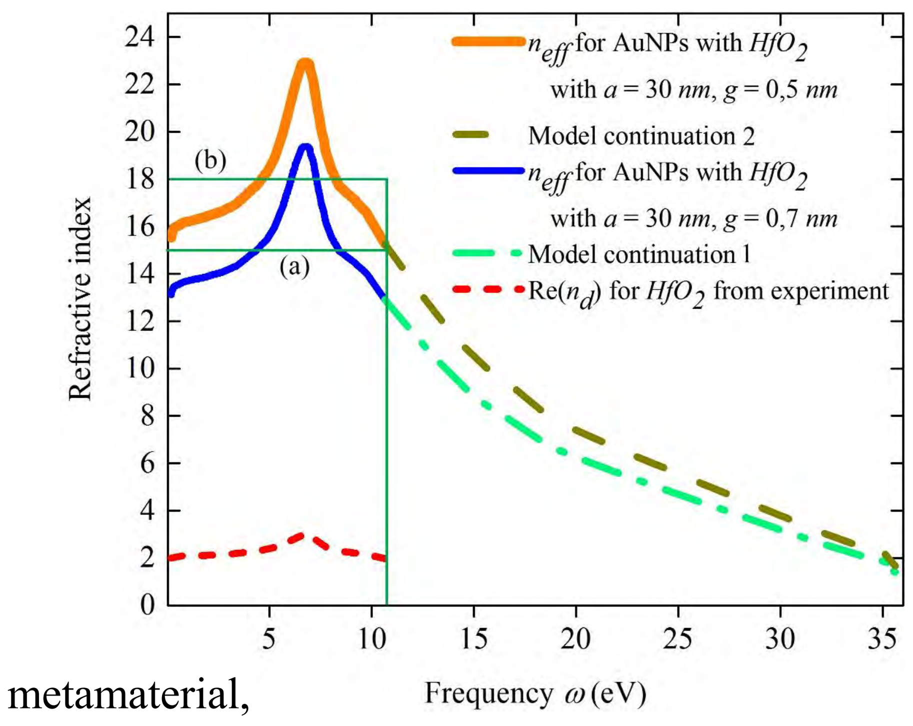
The dependence of absolute value of self-energy correction to the ionization energy of hydrogen atom and alkali metals δE_{ion}^{pc} on the refractive index of the 1D PC structure host.

The effect is strongly enhanced with using hybrid 1D PC with highly tunable refractive index metamaterials as optically dense layers [3].

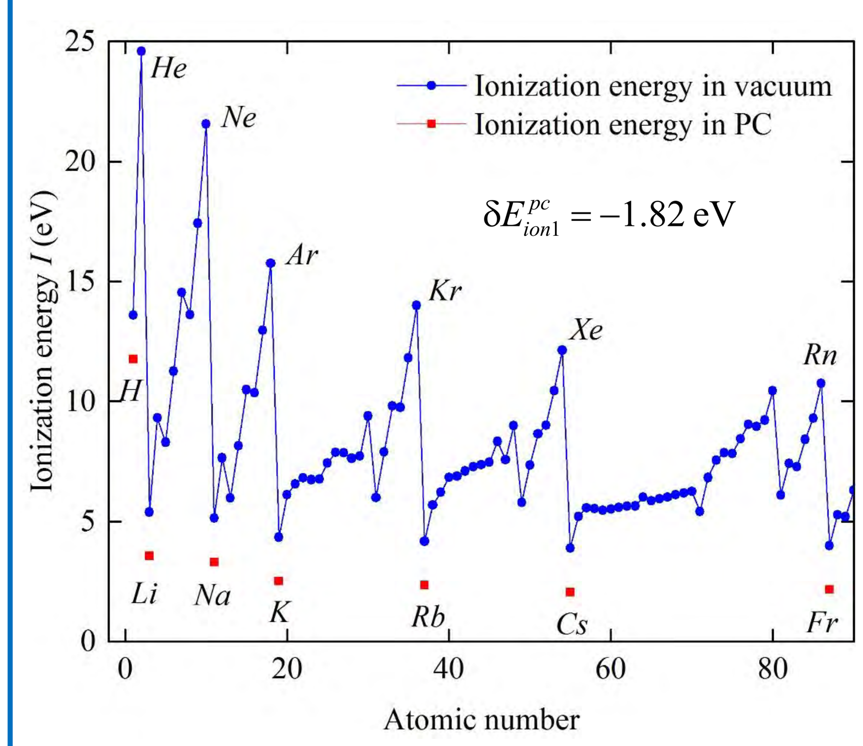
1D PCs on the base of highly tunable refractive index metamaterials and acceleration of chemical reactions

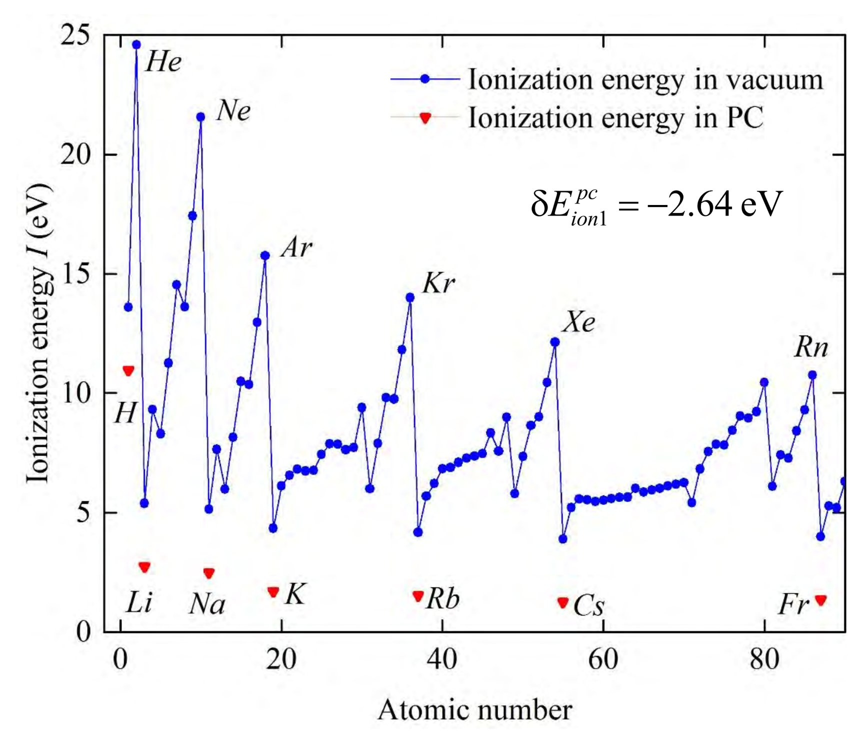


$$n_{eff} = \left(\varepsilon_{eff}\cdot\mu_{eff}\right)^{\frac{1}{2}} \approx \left(\varepsilon_{eff}\right)^{\frac{1}{2}} \approx \left(\varepsilon_h \cdot \frac{a}{g}\right)^{\frac{1}{2}},$$



where n_{eff} is effective refractive index of a metamaterial, ε_h is the permittivity of dielectric metamaterial's host, a, g are the size of particles and gap between them.

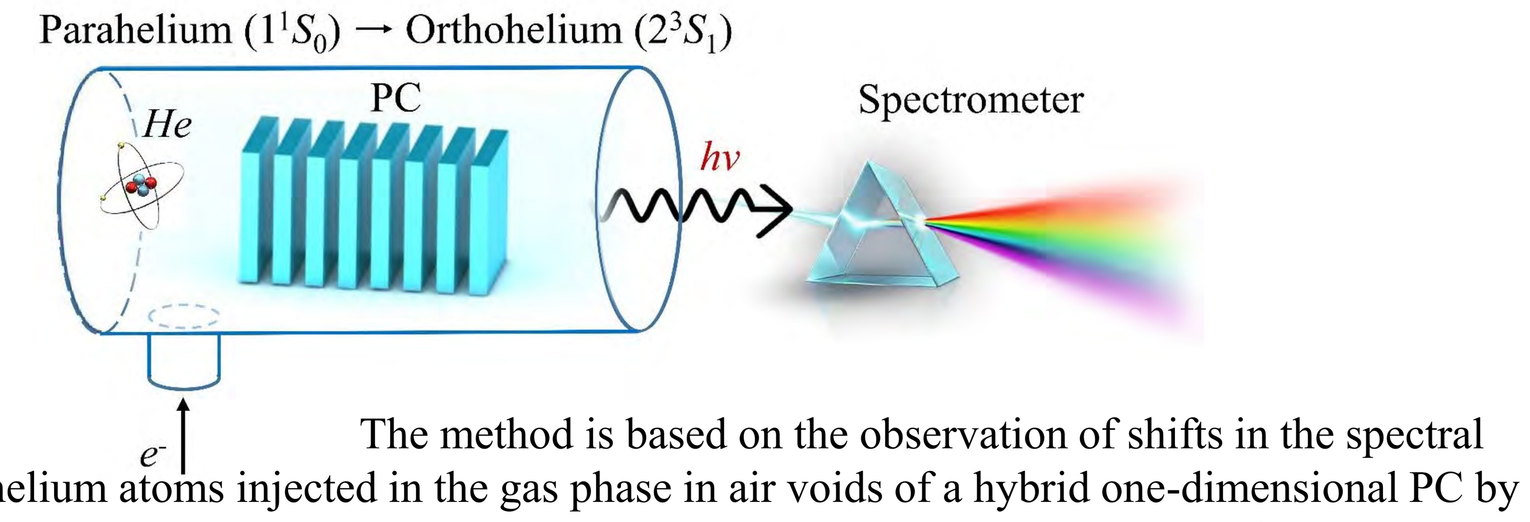




The comparison of ionization energy of hydrogen atom and the alkali metals for the case of vacuum (blue dots) and (a) the PC medium (red squares) on the base of metamaterial with $a = 30$ nm, $g = 0.7$ nm and (b) the PC medium (red triangles) on the base of metamaterial with a = 30 nm, g = 0.5 nm. The ionization energy correction has a value (a) – 1.82 eV and (b) – 2.64 eV.

Schematic of suggested experiment of the verification of the QED effect of the PC correction to the helium electrons masses

Parahelium (1^1S_0) → Orthohelium (2^3S_1)



The method is based on the observation of shifts in the spectral lines of helium atoms injected in the gas phase in air voids of a hybrid one-dimensional PC by optical spectroscopy techniques. The parahelium atoms (with the singlet state 1^1S_0) are excited by an electron beam to the metastable state 2^3S_1 of orthohelium. Transitions between triplet states of the orthohelium atom can be observed due to the long lifetime of this metastable state which is about 7.9 years.

Results and Conclusions:

New artificial materials such as **PCs**, **metamaterials**, having **unique optical properties**, provide the **opportunity** for many **applications** in **photonics**, **chemistry**, **biology** and **quantum technology**, and are the **good testbed system** for the study of the **fundamental QED effects**. **In this work**, the **method** of **experimental verification** of the **QED effect** of the **electromagnetic mass change** of an **electron** in **artificial periodical materials** like **PCs is suggested**. **The experimental verification** of **this QED effect** can be very **interesting** and **significant** from the **fundamental theory** and **possible practical applications**. We believe that **experimental verification** of the **effect** under study can open up **new opportunities** for the **study** of **chemical** and **biochemical reactions** and for the **synthesis** of **exceptional chemical compounds in confined environment** that could be used in **pharmaceutics** and **medical applications**.

References:

1. John, S. Phys. Rev. Lett. 1987. V. 58. P. 2486.
2. Gainutdinov R.Kh., Khamadeev M.A., and Salakhov M.Kh. Phys. Rev. A. 2012. V. 85. 053836.
3. Gainutdinov, R.Kh., Garifullin, A.I., Khamadeev M.A., and Salakhov M.Kh. Phys. Lett. A. 2021. V. 404. P. 127407.