UDC 535.42

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RESONANT AUGER SPECTROSCOPY OF THE ATOMS OF INERT GASES

The results of determination and analysis of the resonant Auger transition spectra characteristics for atoms of the inert gases are obtained within the relativistic multi-body theory and compared with available experimental and other theoretical data. A number of the Auger transition parameters have been firstly presented.

1. INTRODUCTION

The Auger electron spectroscopy remains an effective method to study the chemical composition of solid surfaces and near-surface layers [1—8]. Sensing the Auger spectra in atomic systems and solids gives the important data for the whole number of scientific and technological applications. So called two-step model is used most widely when calculating the Auger decay characteristics [1—5]. Since the vacancy lifetime in an inner atomic shell is rather long (about 10^{-17} to 10^{-14} s), the atom ionization and the Auger emission are considered to be two independent processes. In the more correct dynamic theory of the Auger effect [2, 3] the processes are not believed to be independent from one another. The fact is taken into account that the relaxation processes due to Coulomb interaction between electrons and resulting in the electron distribution in the vacancy field have no time to be over prior to the transition.

In fact, a consistent Auger decay theory has to take into account correctly a number of correlation effects, including the energy dependence of the vacancy mass operator, the continuum pressure, spreading of the initial state over a set of configurations etc [1—19]. The most widespread theoretical studying the Auger spectra parameters is based on using the multi-configuration Dirac—Fock (MCDF) calculation [2, 3]. The theoretical predictions based on MCDF calculations have been carried out within different approximations and remained hitherto non-satisfactory in many relations. Earlier [8—13] it has been proposed relativistic perturbation theory (PT) method of the Auger decay characteristics for complex atoms, which is based on the Gell-Mann and Low S-matrix formalism energy approach) and QED PT formalism [4—7]. The novel element consists in an using the optimal basis of the electron state functions derived from the minimization condition for the calibration-non-invariant contribution (the second order PT polarization diagrams contribution) to the imaginary part of the multi-electron system energy already at the first non-disappearing approximation of the PT. Earlier it has been applied in studying the Auger decay characteristics for a set of neutral atoms, quasi-molecules and solids. Besides, the ionization cross-sections of inner shells in various atoms and the Auger electron energies in solids were estimated. Here we present new results of determination and analysis of the resonant Auger transition spectra characteristics for atoms of the inert gases (Ne, Xe), which are obtained within the relativistic multi-body theory [8—13] and compared with available experimental and other theoretical data. A number of the Auger transition parameters has been firstly presented.

2. THEORETICAL APPROACH TO DETERMINATION OF THE AUGER DECAY CHARACTERISTICS

Within the frame of QED PT approach the Auger transition probability and the Auger line intensity are defined by the square of an electron interaction matrix element having the form [5]:

$$V^{\omega}_{1234} = \left[(j_1)(j_2)(j_3)(j_4)\right]^{1/2} \times \times \sum_{\lambda\mu} (-1)^{\mu} \begin{pmatrix} j_1 j_3 & \lambda \\ m_1 - m_3 & \mu \end{pmatrix} \times \mathrm{Re}\, Q_{\lambda}(1234); \quad Q_{\lambda} = Q^{\mathrm{Qul}}_{\lambda} + Q^{\mathrm{Br}}_{\lambda}. \qquad (1)$$

The terms $Q^{\mathrm{Qul}}_{\lambda}$ and $Q^{\mathrm{Br}}_{\lambda}$ correspond to subdivision of the potential into Coulomb part $\cos|\omega|r_{12}/r_{12}$ and Breat one, $\cos|\omega|r_{12}\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2/r_{12}$. The real part of the electron interaction matrix element is determined using expansion in terms of Bessel functions:

$$\frac{\cos|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \times \times \sum_{\lambda=0} (\lambda) J_{\lambda+1/2}(|\omega| r_<) J_{-\lambda-1/2}(|\omega| r_>) P_{\lambda}(\cos \mathbf{r}_1\mathbf{r}_2), \quad (2)$$

where J is the 1st order Bessel function, $(\lambda) = 2\lambda + 1$. The Coulomb part $Q^{\mathrm{Qul}}_{\lambda}$ is ex-

pressed in terms of radial integrals R_λ, angular coefficients S_λ [4]:

$$\mathrm{Re}\,Q_\lambda^{\mathrm{Qul}} = \frac{1}{Z}\mathrm{Re}\{R_l(1243)S_\lambda(1243) + \\ + R_\lambda(\tilde{1}243)S_\lambda(\tilde{1}24\tilde{3}) + R_\lambda(1\tilde{2}4\tilde{3})S_\lambda(1\tilde{2}4\tilde{3}) + \\ + R_\lambda(\tilde{1}\tilde{2}4\tilde{3})S_\lambda(\tilde{1}\tilde{2}4\tilde{3})\}. \quad (3)$$

As a result, the Auger decay probability is expressed in terms of $\mathrm{Re}Q_\lambda(1243)$ matrix elements:

$$\mathrm{Re}\,R_\lambda(1243) = \\ = \iint \mathrm{d}r_1 r_1^2 r_2^2 f_1(r_1) f_3(r_1) f_2(r_2) f_4(r_2) Z_\lambda^{(1)}(r_<) Z_\lambda^{(1)}(r_>), \quad (4)$$

where f is the large component of radial part of single electron state Dirac function; function Z and angular coefficient are defined in refs. [4—7]. The other items in (3) include small components of the Dirac functions; the sign «$\sim$» means that in (3) the large radial component f_i is to be changed by the small g_i one and the moment l_i is to be changed by $\tilde{l}_i = l_i - 1$ for Dirac number $æ_1 > 0$ and $l_i + 1$ for $æ_i < 0$.

The Breat interaction is known to change considerably the Auger decay dynamics in some cases. The Breat part of Q is defined in [4, 5]. The Auger width is obtained from the adiabatic Gell—Mann and Low formula for the energy shift [5]. The direct contribution to the Auger level width with a vacancy $n_\alpha l_\alpha j_\alpha m_\alpha$ is as follows:

$$\sum_\lambda \frac{2}{(\lambda)(j_\alpha)} \sum_{\beta\gamma \leqslant f} \sum_{k>f} Q_\lambda(\alpha k\gamma\beta) Q_\lambda(\beta\gamma k\alpha), \quad (5)$$

while the exchange diagram contribution is:

$$\frac{2}{(j_\alpha)} \sum_{\lambda_1\lambda_2} \sum_{\beta\gamma \leqslant f} \sum_{k>f} Q_{\lambda_1}(\alpha k\gamma\beta) Q_{\lambda_2}(\beta\gamma k\alpha) \begin{Bmatrix} j_\alpha & j_\gamma & \lambda_2 \\ j_k & j_\beta & \lambda_1 \end{Bmatrix}. \quad (6)$$

The partial items of the $\sum_{\beta\gamma}\sum_{k}$ sum answer to contributions of $\alpha^{-1} \to (\beta\gamma)^{-1}K$ channels resulting in formation of two new vacancies $\beta\gamma$ and one free electron k: $\omega_k = \omega_\alpha + \omega_\beta - \omega_\alpha$. The final expression for the width in the representation of jj-coupling scheme of single-electron moments has the form:

$$\Gamma(2j_1^o l_1^o, 2j_2^o l_2^o; J) = 2\sum_{j_k l_k} |\Gamma(2j_1^o l_1^o, 2j_2^o l_2^o; 1l_o, kjl)|^2. \quad (7)$$

Here the summation is made over all possible decay channels.

Contribution of the main polarization diagrams (the particle-hole interaction) of the second and higher orders of the PT to the energy can be presented as follows:

$$E(A) = \iint \mathrm{d}r_1 \mathrm{d}r_2 \cdot \rho_1(r_1) \cdot V_{\mathrm{pol}}^d(r_1 r_2) \cdot \rho_2(r_2) \quad (8)$$

with effective two-quasiparticle interaction [3]:

$$V_{\mathrm{pol}}^d(r_1 r_2) = X\left\{\int \frac{\mathrm{d}r'(\rho_c^{(0)}(r'))^{1/3}\theta(r')}{|r_1 - r'|\cdot|r' - r_2|} - \right. \\ \left. \int \frac{\mathrm{d}r'(\rho_c^{(0)}(r'))^{1/3}\theta(r')}{|r_1 - r'|} \times \int \frac{\mathrm{d}r''(\rho_c^{(0)}(r''))^{1/3}\theta(r'')}{|r'' - r_2|} \Big/ \langle(\rho_c^{(0)})^{1/3}\rangle\right\},$$

$$\langle(\rho_c^{(0)})^{1/3}\rangle = \int \mathrm{d}r(\rho_c^{(0)}(r))^{1/3}\theta(r), \quad (9)$$

$$\theta(r) = \left\{1 + \frac{\left[3\pi^2 \cdot \rho_c^{(0)}(r)\right]^{2/3}}{c^2}\right\}^{1/2},$$

where ρ_c^0 is the core ("Fermi sea") electron density (without quasiparticles), X is the numerical coefficient, c is the velocity of light. The similar potential representation can be obtained for the exchange polarization quasiparticle interaction (see details in ref. [3, 11, 13]).

The basis of the particle state functions is defined by the solution of the Dirac—Fock equation (integrated numerically using the Runge—Cutt method). Novel element is connected with using ab initio paoptimized Dirac—Fock potential with the formal parameter which is determined on the basis of the QED optimization procedure (see details in refs. [4—6, 11, 13]).

The calculation of radial integrals $\mathbf{Re}\,R_\lambda(1243)$ is reduced to the solution of a system of differential equations [5]:

$$y_1' = f_1 f_3 Z_\lambda^{(1)}(\alpha|\omega|r) r^{2+\lambda}; \\ y_2' = f_2 f_4 Z_\lambda^{(1)}(\alpha|\omega|r) r^{2+\lambda}; \quad (8) \\ y_3' = [y_1 f_2 f_4 + y_2 f_1 f_3] Z_\lambda^{(2)}(\alpha|\omega|r) r^{1-\lambda}.$$

In addition,

$$y_3(\infty) = \mathbf{Re}\,R_\lambda(1243), \; y_1(\infty) = X_\lambda(13).$$

The formulae for the Auger decay probability include the radial integrals $R_\alpha(\alpha k\gamma\beta)$, where one of the functions describes electron in the continuum state. The energy of an electron formed due to a transition jkl is defined by the difference between energies of atom with a hole at j level and double-ionized atom at kl levels in final state:

$$E_A(jkl, {}^{2S+1}L_J) = E_A^+(j) - E_A^{2+}(kl, {}^{2S+1}L_J). \quad (10)$$

To single out the above-mentioned correlation effects, the equation (12) can be presented as [8, 9]:

$$E_A(jkl, {}^{2S+1}L_J) = E(j) - E(k) - E(l) - \\ - \Delta(k, l; {}^{2S+1}L_J), \quad (11)$$

where the item Δ takes into account the dynamic correlation effects (relaxation due to hole screening with electrons etc.) To take these effects into account, the set of procedures elaborated in the atomic theory [8—13] is used.

3. RESULTS AND CONCLUSIONS

In tables 1 we present the data on the transition energies and angular anisotropy parameter β (for each parent state) for the resonant

Auger decay to the $2s^12p^5(^{1,3}P)$ np and $2s^0p^6\ ^2S$ np ($n = 3,4$) states of Ne^+. There are listed the experimental data by De Fanis et al [18] and Pahler et al [15], theoretical ab initio Hartree-Fock results [18] and our data, obtained within the relativistic many-body PT with using the gauge-invariant QED PT method for generating relativistic functions basis's. In table 2 we the data on the widths (meV) for the $2s^12p^5(^{1,3}P)np$ and $2s^0p^6\ (^1S)$ np ($n = 3,4$) slates of Ne^+. There are listed the experimental data by [18], theoretical ab initio multi configuration Hartree—Fock results by Sinanis et al [16], single-configuration Hartree-Fock data by Armen—Larkins [17] and our data, obtained within the relativistic many-body PT.

In table 3 we present data on the initial and final states of the most intense $4d^{-2} \to 4d^{-1} \to 5p^{-2}$ and $4d^{-1}5p^{-2} \to 5p^{-4}$ Auger transitions in the neutral xenon. The calculated intensities are given relative to the creation of one 3d hole, and only intensities $\geqslant 0.005$ are listed. Our theoretical data (the relativistic many-body PT) and the theoretical pseudorelativistic Hartree Fock data by Jonauskas et al [19], semiempirical (with using the Cowan code) [20] and experimental [19] kinetic energies of the Auger transitions are also given.

Table 1

Transition energies E_k, angular anisotropy parameters β (for each parent state for the resonant Auger decay to the $2s^12p^5(^{1,3}P)$ np and $2s^0p^6\ ^2S$ np ($n = 3,4$) states of Ne^+: the experimental data [18, 15], theoretical *ab initio* Hartree—Fock results [18] and our data, obtained within the relativistic many-body PT

Final state	Exp. E_k, [18]	Theory: E_k, [18]	Theory: E_k, our	β; Exp. [18]	Theory: β, [18]	Theory: β — our data
$2s^12p^5(^1P)3p\ ^2S$	778.79	776.43	778.52	1.7 ± 0.3	2.000	1.832
$2s^12p^5(^1P)3p\ ^2P$	778.54	776.40	778.27	-0.94 ± 0.06	−0.996	−0.959
$2s^12p^5(^1P)3p\ ^2D$	778.81	776.66	778.57	0.20 ± 0.06	0.200	0.202
$2s^12p^5(^1P)3p\ ^2S$	788.16	786.51	787.88	1.5 ± 0.1	1.998	1.678
$2s^12p^5(^1P)3p\ ^2P$	788.90	787.52	788.69	-0.91 ± 0.06	−0.928	−0.916
$2s^12p^5(^1P)3p\ ^2D$	789.01	787.64	788.82	0.06 ± 0.05	0.156	0.074
$2s^12p^5(^1P)4p\ ^2S$	773.60		773.48	0.96 ± 0.28		0.972
$2s^12p^5(^1P)4p\ ^2P$	773.48		773.25	-0.92 ± 0.06		−0.928
$2s^12p^5(^1P)4p\ ^2D$	773.56		773.33	0.15 ± 0.06		0.156
$2s^12p^5(^3P)4p\ ^2S$	783.72		783.54	1.97 ± 0.40		2.045
$2s^12p^5(^3P)4p\ ^2P$	783.95		783.78	-0.43 ± 0.09		−0.444
$2s^12p^5(^3P)4p\ ^2D$	784.01		783.82	0.09 ± 0.20		0.102
$2s^02p^6(^1S)3p\ ^2P$	—		754.93	0.05 ± 0.14		0.061
$2s^02p^6(^1S)4p\ ^2P$	—		749.85	0.07 ± 0.18		0.082

Table 2

Widths (meV) for the $2s^12p^5(^{1,3}P)np$ and $2s^0p^6\ (^1S)$ np ($n = 3,4$) slates of Ne^+: the experimental data [18], theoretical *ab initio* multi configuration Hartree—Fock results by Sinanis et al [16], single-configuration Hartree—Fock data by Armen—Larkins [17] and our data, obtained within the relativistic many-body PT

final state	Exp. [18]	Exp. [15]	Theory [17]	Theory [16]	Theory: Our data
$2s^12p^5(^1P)3p\ ^2S$	530 ± 50	410 ± 50	687	510	524
$2s^12p^5(^1P)3p\ ^2P$	42 ± 3	—	20.7	—	38
$2s^12p^5(^1P)3p\ ^2D$	34 ± 4	—	40.2	—	32
$2s^12p^5(^3P)3p\ ^2S$	120 ± 10	110 ± 40	18.8	122	118
$2s^12p^5(^3P)3p\ ^2P$	19 ± 5	—	10.3	—	16
$2s^12p^5(^3P)3p\ ^2D$	80 ± 10	—	62.3	—	72
$2s^12p^5(^1P)4p\ ^2S$	135 ± 20	—	—	—	121
$2s^12p^5(^1P)4p\ ^2P$	—		—	—	3
$2s^12p^5(^1P)4p\ ^2D$	—	—	—	—	8
$2s^12p^5(^3P)4p\ ^2S$	—	—	—	—	27
$2s^02p^6(^1S)3p\ ^2P$	80 ± 5	—	—	—	78
$2s^02p^6(^1S)4p\ ^2P$	20 ± 3	—	—	—	18

Table 3

Calculated and experimental intensities I, kinetic energies E_k for Xe *(see text)*

	Initial state	Final state	I [19]	I, our	Theor E [19]	Theor E, our	Theor E [20]	Exp. [19]
a	$4d^{-2}\ {}^1G_4\rightarrow$	$4d^{-1}\ 5p^{-2}({}^1D)\ {}^2F_{5/2}$	0.005	0.006	31.5	31.3		}
a	$4d^{-2}\ {}^1G_4\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^3P)\ {}^2F_{7/2}$	0.013	0.014	31.2	31.0		} 30.8
a	$4d^{-2}\ {}^1G_4\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^1D)\ {}^2G_{9/2}$	0.009	0.010	30.9	30.6		}
b	$4d^{-2}\ {}^1D^2\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^3P)\ {}^2D_{5/2}$	0.005	0.006	30.5	30.3		30.3
c	$4d^{-2}\ {}^1G_4\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^3P)\ {}^2D_{3/2}$	0.007	0.007	30.1	30.0		29.9
d	$4d^{-2}\ {}^1G_4\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^1D)\ {}^2D_{5/2}$	0.005	0.006	29.3	29.2		}
d	$4d^{-2}\ {}^1D_2\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^1D)\ {}^2F_{7/2}$	0.008	0.009	29.1	29.1		} 29.1
d	$4d^{-2}\ {}^1G_4\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^1D)\ {}^2F_{7/2}$	0.008	0.009	29.1	29.1		}
d	$4d^{-2}\ {}^3F_4\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^3P)\ {}^4F_{9/2}$	0.006	0.007	29.1	29.1		}
e	$4d^{-2}\ {}^3F_4\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^3P)\ {}^4F_{5/2}$	0.007	0.006	28.4	28.3		
e	$4d^{-2}\ {}^3F_4\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^3P)\ {}^2F_{5/2}$	0.005	0.005	28.1	28.0		} 28.3
f	$4d^{-2}\ {}^1G_4\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^1S)\ {}^2D_{5/2}$	0.018	0.019	27.8	27.8		27.9
g	$4d^{-2}\ {}^3F_2\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^1D)\ {}^2G_{9/2}$	0.005	0.006	27.4	27.3		} 27.1
g	$4d^{-2}\ {}^3P_1\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^1S)\ {}^2D_{5/2}$	0.005	0.006	27.0	26.9		
h	$4d^{-2}\ {}^3F_4\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^3P)\ {}^2F_{5/2}$	0.008	0.009	26.5	26.5		}26.5
h	$4d^{-2}\ {}^1D_2\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^1S)\ {}^2D_{3/2}$	0.009	0.010	26.1	26.2		
h	$4d^{-2}\ {}^1G_4\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^1S)\ {}^2D_{3/2}$	0.008	0.008	26.1	26.2		
h	$4d^{-2}\ {}^3P_2\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^1S)\ {}^2D_{5/2}$	0.006	0.006	25.9	26.0		
i	$4d^{-2}\ {}^3F_4\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^1D)\ {}^2G_{9/2}$	0.008	0.008	25.6	25.9		—
j	$4d^{-2}\ {}^3F_2\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^1S)\ {}^2D_{5/2}$	0.005	0.006	24.3	24.6		24.7
k	$4d^{-2}\ {}^3F_4\rightarrow$	$4d^{-1}\ 5p^{-2}\ ({}^1S)\ {}^2D_{5/2}$	0.006	0.007	22.5	22.9		
l	$4d^{-1}\ 5p^{-2}({}^1S)\ {}^2D_{3/2}$	$5p^{-4}\ {}^1D_2$	0.010	0.010	20.8	20.9	20.9	21.0
m	$4d^{-1}\ 5p^{-2}({}^1S)\ {}^2D_{5/2}$	$5p^{-4}\ {}^1D_2$	0.021	0.022	19.2	19.3	19.5	}19.3
m	$4d^{-1}\ 5p^{-2}({}^1D)\ {}^2S_{1/2}$	$5p^{-4}\ {}^1D_2$	0.005	0.006	18.9	19.0	18.9	
n	$4d^{-1}\ 5p^{-2}({}^1S)\ {}^2D_{3/2}$	$5p^{-4}\ {}^1S_0$	0.014	0.015	18.3	18.7	18.9	18.9
o	$4d^{-1}\ 5p^{-2}({}^1D)\ {}^2P_{3/2}$	$5p^{-4}\ {}^1D_2$	0.009	0.009	17.9	18.3		
o	$4d^{-1}\ 5p^{-2}({}^3P)\ {}^4D_{5/2}$	$5p^{-4}\ {}^3P_0$	0.017	0.018	17.9	18.3		
o	$4d^{-1}\ 5p^{-2}({}^3P)\ {}^2F_{5/2}$	$5p^{-4}\ {}^3P_1$	0.005	0.005	17.8	18.2		} 18.6
o	$4d^{-1}\ 5p^{-2}({}^3P)\ {}^2F_{7/2}$	$5p^{-4}\ {}^3P_2$	0.011	0.012	17.7	18.1		
o	$4d^{-1}\ 5p^{-2}({}^1D)\ {}^2D_{5/2}$	$5p^{-4}\ {}^1D_2$	0.009	0.009	17.6	18.0	18.4	
p	$4d^{-1}\ 5p^{-2}({}^3P)\ {}^2F_{5/2}$	$5p^{-4}\ {}^3P_2$	0.006	0.007	17.1	17.6		
q	$4d^{-1}\ 5p^{-2}({}^1S)\ {}^2D_{5/2}$	$5p^{-4}\ {}^1S_0$	0.017	0.017	16.7	17.3	17.5	} 17.5
q	$4d^{-1}\ 5p^{-2}({}^3P)\ {}^2D_{5/2}$	$5p^{-4}\ {}^1D_2$	0.009	0.009	16.4	17.0		
r	$4d^{-1}\ 5p^{-2}({}^1D)\ {}^2G_{9/2}$	$5p^{-4}\ {}^1D_2$	0.020	0.021	16.0	16.6	16.6	16.6
s	$4d^{-1}\ 5p^{-2}({}^3P)\ {}^2F_{7/2}$	$5p^{-4}\ {}^1D_2$	0.008	0.009	15.7	16.3		
s	$4d^{-1}\ 5p^{-2}({}^1D)\ {}^2F_{7/2}$	$5p^{-4}\ {}^1S_0$	0.005	0.005	15.4	15.9		
s	$4d^{-1}\ 5p^{-2}({}^3P)\ {}^2F_{5/2}$	$5p^{-4}\ {}^1D_2$	0.005	0.005	15.2	15.7		
t	$4d^{-1}\ 5p^{-2}({}^3P)\ {}^2D_{3/2}$	$5p^{-4}\ {}^1S_0$	—	0.005	—	14.9		
u	$4d^{-1}\ 5p^{-2}({}^1D)\ {}^2G_{9/2}$	$5p^{-4}\ {}^1S_0$	—	0.006	—	14.1		

The analysis of the presented results in tables 1—3 allows to conclude that the précised description of the Auger processes requires the detailed accurate accounting for the exchange-correlation effects, including the particle-hole interaction, screening effects and iterations of the mass operator. The relativistic many-body PT approach provides more accurate results that is due to a considerable extent to more correct accounting for complex inter electron exchange-correlation effects. It is important to note that using the more correct gauge-invariant procedure of generating the relativistic orbital basis's directly linked with correctness of accounting

for the correlation effects. The same is regarding the procedure of accounting the relativistic effects (especially for Xe).

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UDC 535.42

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RESONANT AUGER SPECTROSCOPY OF THE ATOMS OF INERT GASES

Abstract

The results of determination and analysis of the resonant Auger transition spectra characteristics for atoms of the inert gases are obtained within the relativistic multi-body theory and compared with available experimental and other theoretical data. A number of the Auger transition parameters have been firstly presented.

Key words: Auger spectroscopy, atom of inert gas, relativistic theory

УДК 535.42

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РЕЗОНАНСНАЯ ОЖЕ СПЕКТРОСКОПИЯ АТОМОВ ИНЕРТНЫХ ГАЗОВ

Резюме

Представлены результаты теоретического определения в рамках релятивистской многочастичной теории и анализа характеристик резонансных спектров Оже переходов для атомов инертных газов и проведено их сравнение с имеющимися экспериментальными и альтернативными теоретическими данными. Для ряда Оже переходов характерные параметры получены впервые.

Ключевые слова: Оже спектроскопия, атом инертного газа, релятивистская теория.

УДК 535.42

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РЕЗОНАНСНА ОЖЕ СПЕКТРОСКОПІЯ АТОМІВ ІНЕРТНИХ ГАЗІВ

Резюме

Наведені результати теоретичного визначення у межах релятивістської багаточастинкової теорії та аналізу характеристик резонансних спектрів Оже переходів для атомів інертних газів і проведено їх порівняння з наявними експериментальними та альтернативними теоретичними даними. Для ряду Оже переходів характерні параметри отримані вперше.

Ключові слова: Оже спектроскопія, атом інертного газу, релятивістська теорія.