ORIGIN OF THE LOW LIFETIMES FOR THE LOCALIZED o-PS IN THE LARGE PORES OF POROUS MATERIALS: A NEW FINDING BY THE COMBINATION MODEL OF QUANTUM AND SEMI-CLASSICAL PHYSICS

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Abstract: Positron annihilation is of great interest for applications in evaluating material structures in range from a few angstroms to hundreds of nanometers. Here, we report on a new model for calculating the free volume size in porous materials from the experimental ortho-Positronium (o-Ps) lifetimes reported and updated over than past four decades by the combination of the quantum and semi-classical physics models. By proposing the o-Ps diffusion probability parameter (D) from the pore to the virtual electron layer (ΔR) of material and considering the simultaneous effect of the pore surface area and the mean free path of o-Ps in the pore for the average value of D, we have successfully built the simply model for the different pore geometries including channels, spheres and ellipsoids. Moreover, we have found and elucidated for the first time the origin of the low lifetimes of o-Ps in the large pores by forecasting the elliptic geometry which were not well understood in past two decades. The present model' salient features in comparison with the previously different models is the value of ΔR = 0.166 nm can be utilized to calculate the pore size in the universal range of 0.2 - 400 nm for almost all porous materials.

Keywords: *Positron, o-Ps lifetime , porous material, physiscal model.*

1. INTRODUCTION

Controlling and salvaging reciprocal influences between porosity, crystal structure, lattice defects, surface property, molecular transport, and reaction in functional materials are keys to various technologies for sustainable development of the world [1] Nanostructured material such as silica, zeolite, metal-organic framework material, etc. contain a complex matrix of pore structures which plays a core role to their applications in environmental treatments, industrial catalysis and energy storage, etc. In the structural research of the above materials, the applicable limitations of adsorbed/desorbed methods at the nanometer scale lead to participation of the nuclear methods such as the small angle neutron scattering (SANS) and Positron annihilation lifetime spectroscopy (PALS) [2-4]. In reality, PALS was applied for studies on material structure in the last many decades [5-10]. One of the most obvious applications arises from the fact that, in material, structural traps as micro/mesopores (channels, cavities or cages), defects (vacancies, voids, etc.) the influence on the local electron distributions could significantly change positron lifetimes [8,10]. Consequently, the localized o-Ps lifetime is sensitive to the trap size, that is, the larger the trap, the longer lifetime of the localized o-Ps [5]. For the spherical pores, the first and simplest model describing the correlation of o-Ps lifetime ($1/\lambda$) and pore radius (R) through pick-off annihilation was proposed by Tao and Eldrup (TE model) with the infinite deep well [11]. This model was only suitable for pores smaller than 1 nm [3, 11]. The TE model was improved for the extension of calculating range for the larger pores by modifying the potential well to finite spherical, cylindrical and rectangular geometries or completely approaching from classical mechanics [12-17]. In these studies, the o-Ps excited states, the temperature and the 3γ intrinsic annihilation of o-Ps were considered. However, while the modified models still disagree with

the experimental o-Ps lifetimes for large pores [12, 13, 16] or to be complex for applications [15] then classical models fail for small pores (R_0 <1 nm) [14] or to be only specific for measurements in air [17].

In this paper, we report on a new model for calculating the universal free volume size in porous materials from the experimental o-Ps lifetime by combining of quantum and semi-classical physics models. To determine the model parameters, the experimental data of the o-Ps lifetimes in porous materials reported and updated over than past four decades are used. In order to verify the correctness of the model, the o-Ps lifetimes in the channel pores of porous materials are employed.

2. THE PHYSICAL MODEL FOR o-PS IN LARGE PORES

Firstly, in consideration of the TE model, the pick-off annihilation rate of o-Ps depending on only the pore radius was presented by:

$$\lambda_{TE} = \lambda_0 . f_{TE}(R) \tag{1}$$

$$f_{TE}(R) = [1 - \frac{R_0}{R_0 + \Delta R} + \frac{1}{2\pi} \sin(2\pi \frac{R_0}{R_0 + \Delta R})] \tag{2}$$

where, $\lambda_0 = \pi r_0^2 c \rho_0$ is the decay rate of o-Ps in the virtual electron layer (ΔR), r_0 is the classical radius of the electron, c is the velocity of light, ρ_0 is the electron density at the o-Ps site, R_0 is the pore radius and $\Delta R = R - R_0$ (≈ 0.166 nm) which depicts the overlap of o-Ps and electron wave-functions at the wall of pores [11]. In the small radius region of pores (R_0 < 1nm), o-Ps is confined in an infinite potential well. The state of o-Ps, in this case, is presented by a standing wave (Fig. 1. a).

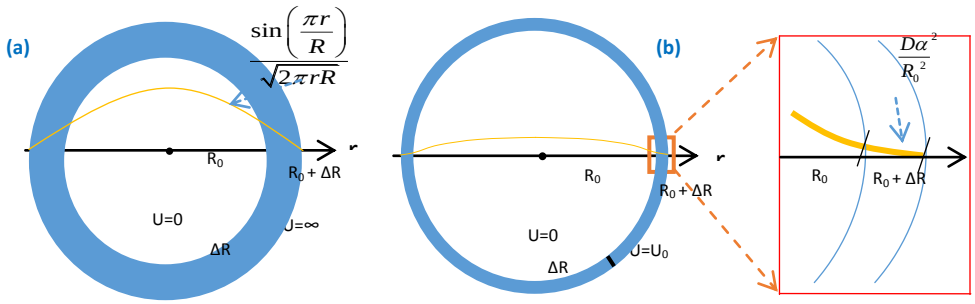

FIG. 1. (a) The Tao-Eldrup model for o-Ps in small pores with the spherically symmetric infinite potential well. (b) The semi-classical model for o-Ps in large pores with spherically the symmetric finite potential well.

However, when the pore becomes larger, its radius moves toward the semi-classical region [21]. Here, the o-Ps energy (E) is in range of kT at room temperature (k = Boltzmann constant, T = sample temperature) with the appearance of the low energy levels in the potential well [18]. As a result, o-Ps having lower energy will exist with a longer lifetime which lead to the larger the pore size, the higher the de-trapping probability of o-Ps from [18-21]. Therefore, instead of using the infinitely deep well as the TE model, we proposed the semi-classical model (SE model) describing interaction of o-Ps in the spherically symmetric finite potential well of the energy depth U_0 (Fig. 1. b). In the proposed model, because of the extension of the pore size, the standing wave-function becomes to be not suitable for representing the o-Ps state in the potential well that should be replaced by a Gaussian wave packet scattering back and forth between the energy barriers on the pore wall before annihilating with an electron here [13]. Consequently, the annihilation process of o-Ps can occur through both of the intrinsic annihilation in vacuum at the region around the center of the pore and the pick-off annihilation at the pore wall. When the pore size increases to a large enough space, the o-Ps probability density function becomes almost uniform in the pore and ΔR is very small in comparison with R_0 [21]. For this reason, we assumed that the o-Ps wave-function in the range from R_0 to $R_0 + \Delta R$ (Fig. 1. b) is to be approximated by:

$$\psi_{Se}(r) = D\alpha^2 / R_0^2 \tag{3}$$

where, α is the normalization factor and D proposed as a new parameter of the model is the o-Ps diffusion probability from pore to the virtual electron layer ΔR of material (the o-Ps diffusion probability). Using the normalization conditions for calculating [21], the annihilation rate (λ_{SE}) of o-Ps of the SE model can be expressed as:

$$\lambda_{SE} = \lambda_p . f_{SE}(R_0) \tag{4}$$

$$\lambda_p = \frac{3D}{1+D}\pi r_0^2 c\rho_0 \tag{5}$$

$$f_{SE}(R_0) = \frac{\Delta R}{R_o + \Delta R}\left(\frac{R_0}{R_o + \Delta R}\right)^2 \tag{6}$$

Equations (4), (5) and (6) indicate that the pick-off annihilation rate (λ_{SE}) of the SE model is dependent on not only the pore radius but also the o-Ps diffusion probability. Additionally, interesting points in both the mathematical representation and the physical meaning are described in the equation (1) and (4). In general consideration, both equations above are essentially based on the integration of the characteristic positron annihilation rates (λ_o, λ_p) and the pore size-correlation functions ($f_{TE}(R_0)$, $f_{SE}(R_0)$). It should be noted that λ_o and λ_p describe the o-Ps decay rate in the virtual electron layer ΔR of the TE and SE models, respectively. Hence, the following expression represents the relation between $\boldsymbol{\lambda}_o$ and $\boldsymbol{\lambda}_p$.

$$\lambda_p = \frac{3D}{1+D}\lambda_0 \tag{7}$$

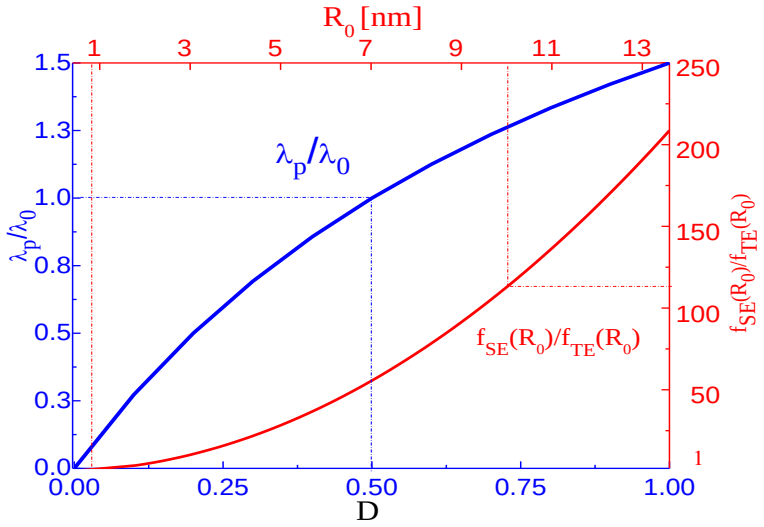

FIG. 2. The plot of the relation between $\boldsymbol{\lambda}_o$ and $\boldsymbol{\lambda}_p$ as well as $f_{TE}(R_0)$ and $f_{SE}(R_0)$.

3. RESUTS AND DISSCUSION

In our previous report [21], D was considered as the o-Ps diffusion coefficient represented by $D \approx \exp(-k.\Delta R)$ for general material, where $k = \sqrt{4m_e(U_0 - E)/\hbar^2}$, m_e is the electron mass and $\hbar$ is the Plank constant. The approximation of D (0.133) was necessary to find simply its value because of the lack of experimental data for the fitting [21]. In the present study, we consider D as the o-Ps diffusion probability to the virtual electron layer ΔR. Consequently, there is a closed relationship of the o-Ps decay rates in TE and the SE models. Within the description of the equation (7), depending on D the o-Ps decay rate in the SE model can vary to be smaller or higher than that in the TE model. Accordingly, the o-Ps decay rates in two models will be balanced $\lambda_o = \lambda_p$ at $D = 0.5$ as indicated in Fig. 2. Hence, the SE model predicts that: if a material has characteristics to satisfy the balanced condition of the back scattering and diffusion probability after each collision of an o-Ps at the pore wall then the o-Ps annihilation rate is only dependent on the pore radius represented by:

$$\lambda_{SE} = \lambda_0 . f_{SE}(R_0) \tag{8}$$

In consideration of the pore size-correlation functions, Fig. 2 and Fig 3 indicate that: *i)* in the case of $R_o \leq 0.7$ nm, values of $f_{TE}(R_0)$ are lower than that of $f_{SE}(R_0)$ resulting in o-Ps lifetimes of the SE model are higher than that of the TE model *ii)* when $R_0 > 0.7$ nm, the ratio of $f_{TE}(R_0)$ and $f_{SE}(R_0)$ rapidly increases versus R_0, which is more than two orders of magnitude at $R_0 = 10$ nm. This is a striking result which predicts that the o-Ps lifetime in the SE model will reach the extreme value in a slower manner compared to the TE model and thus the calculating limitation of the SE model will be more extensive in relation to the TE model. In other words, the TE model is suitable for the small pores, while the SE model is necessary for the large pores. Hence, we propose to combine the two models (the Comb model) for the universal range of the pore size in material by weighting of λ_{TE} and λ_{SE} which take in account the intrinsic annihilation rate λ_T:

$$\lambda_{Comb} = \{[(\lambda_{TE}\lambda_{SE})^{1/2} + \lambda_T][(\lambda_T + \lambda_{TE})(\lambda_T + \lambda_{SE})]^{1/2}\}^{1/2} \qquad (9)$$

The equation (9) can be represented approximately by:

$$\lambda_{Comb} \approx [(2\lambda_{TE} + \lambda_T)(\frac{\lambda_{SE}}{2} + \lambda_T)]^{1/2} \qquad (10)$$

In the SE model, value of D will depend on the kind of material and should be found by fitting experimental data in a wide and diversified range of pore radius. However, result exhibits that the maximum value of λ_p is the one and half of λ_o which occurs when the o-Ps diffusion probability is total (Fig. 2). Furthermore, an important result has been found in the λ_{SE} model that λ_p is affected by not only the pore radius but also the o-Ps diffusion probability. This suggests that for the small pores in material, o-Ps interacts and strongly diffuses to the virtual electron layer which lead to increase of the pick-of annihilation rate and decrease of the o-Ps lifetime as indicated by the TE model. However, when the pore size is large enough, o-Ps could diffuse to the virtual electron layer at the wall resulting in the pick-off annihilation process by emission of 2γ or scatter back the center of pore before appearing the 3γ intrinsic annihilation phenomenon (lifetime of 142 ns for o-Ps decays in vacuum). Thus, the TE model indicates that the intrinsic annihilation rate of o-Ps is a very important factor. However, this factor was not considered by the TE model, formerly.

Fig. 3 describes the dependence of the o-Ps lifetime on the pore radius for the TE (red) and SE (black) models and the fitting curve (blue) of the Comb model. The value of $D = 0.110$ has been examined by fitting the experimental o-Ps lifetimes of porous materials. Results show that the Comb model can very successfully predict for pore sizes. Specially, this model has been expanded for the universal range from 0.2 - 400 nm which are ten times wider than the result reported in our previous study [21] as indicated in Fig. 3.

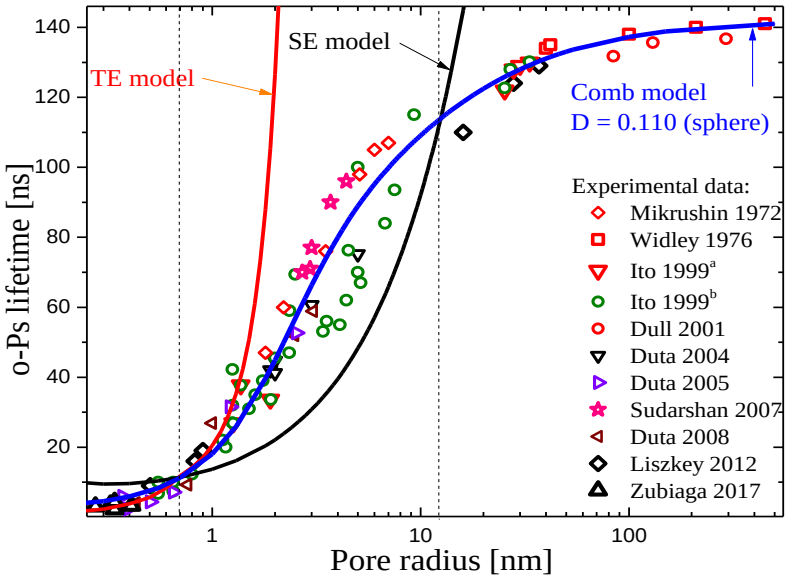

FIG. 3. The TE, Se, Comb models and experimental data for porous materials [4, 13, 15, 16, 17, 20, 22, 23, 24, 25, 26] (a: ref. 13 and b: ref. 25).

However, the value of D fitted from experimental data in Fig. 3 is based on the assumption of the spherical pore. In reality, the pore shapes were almost undefined which can contain the confusedly various geometries.

The influence of the pore geometries on the o-Ps lifetime had been indicated by many earlier published works that discussed the basic geometries such as channels (cylinders), spheres, cubes and cuboids [12, 14, 15], The apparent most successful model to this time was been reported by Dull et al. [15] for rectangular pores (RTE model) by extending the TE model. To reduce complexity of the RTE model, Wada et al. simplified its formulae by proposing a divergent approach to the classical region [27]. However, limitation of the RTE and other models has been a stumbling point as they fail to explain the large amount of experimental data [15, 27] (the low lifetimes as reported by Ito et al. [13, 25], and recently, by Liszkay et al. [14] and Dull et al. [10]). Moreover, the dependence (uncertainty) of ΔR varying in the range of 0.15 - 0.19 on users is the other limitation of the RTE model [12, 15, 16, 26].

To understand the inadequacy of the RTE and other models, it should be noted that the models ignored the low lifetimes of o-Ps in the larger pores in the fitting process [15, 27]. Meanwhile, as indicated in Fig. 3, the experimental lifetimes of o-Ps seem to be separated into three parts: the high lifetimes (data above the Comb curve) which is described well by the RTE model [15]; the medium lifetimes (data near the Comb curve for spherical geometry); and the low lifetimes which appear below the Comb curve. We assume that, the above difference of o-Ps lifetimes originates from the transfer of the spherical pore into the different geometrics such as channels and ellipsoids. Earlier, Goworek indicated the influence of only the mean free paths, which are relative to radius of a pore, on the o-Ps lifetime [28]. However, we propose that when the pore shape changes to the different geometries, the pore surface area (which is closely related to the virtual electron layer ΔR) could become an important parameter for contributions to the change of the o-Ps lifetime. Therefore, we suggest to consider the simultaneous effect of the mean free path of o-Ps in the pore described through radius and the surface area to the change of the o-Ps lifetime. Fig. 4 describes the transfer of a spherical pore into the channel and elliptic pores in the material. Whereby, the value of D for a specified geometry is the average diffusion probability in every direction of the pore:

$$D_{ch} = D_s \frac{S_{ch}(RRR_{ch})^2}{S_s(RRR)^2} \tag{11}$$

$$D_e = D_s \frac{S_e(RR_{e1}R_{e2})^2}{S_s(RRR)^2} \tag{12}$$

where, D_{ch}, D_e, S_{ch} and S_e are o-Ps the diffusion probabilities and the areas of channel and ellipsoid, respectively. Considering to a unit geometry, D_{ch} = 0.066 and D_e = 0.253 (radius of $R_{e1} = R$; $R_{e2} = ¼\ R$ *và* $R_{e3} = 4R$ for ellipsoid) are calculated. It should be noted that, for the elliptic pores, the value of D_{ellip} dependents on the change of the short radius.

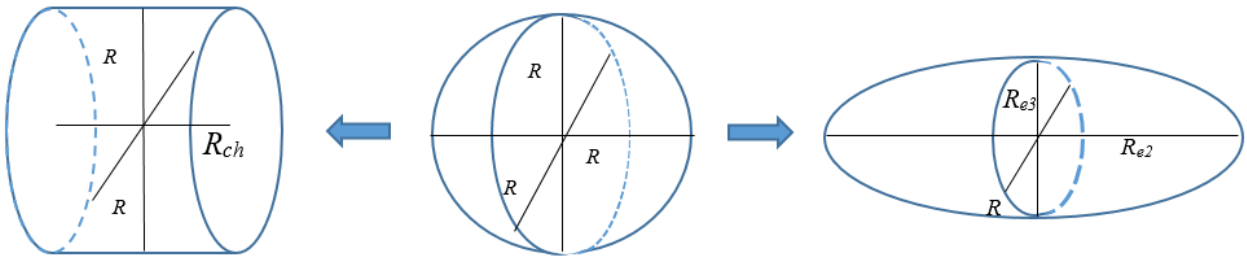

FIG. 4. The transfer of the pore geometries: (a) sphere, (b) channel, and (c) ellipsoid.

Results indicate that the Comb model can well predict o-Ps lifetimes which are in accordance with experimental data for all three pore geometries as indicated in Fig. 5. Whereby, due to decrease of the average diffusion probability, the o-Ps lifetime in the channel pores becomes higher than that in the spherical pore. Conversely, an increase of the average diffusion probability leads to the o-Ps lifetime in the elliptic pore to be lower than that in the spherical pore. These consequences of the Comb model for different pore geometries are suitable with results reported in Ref. 28 and 29. Therefore, the low lifetimes reported by Ito et al. [13, 25], Liszkay et al. [24] and Dull et al. [10] should originate from the elliptic pores which was not considered and explained by the RTE and other models, formerly.

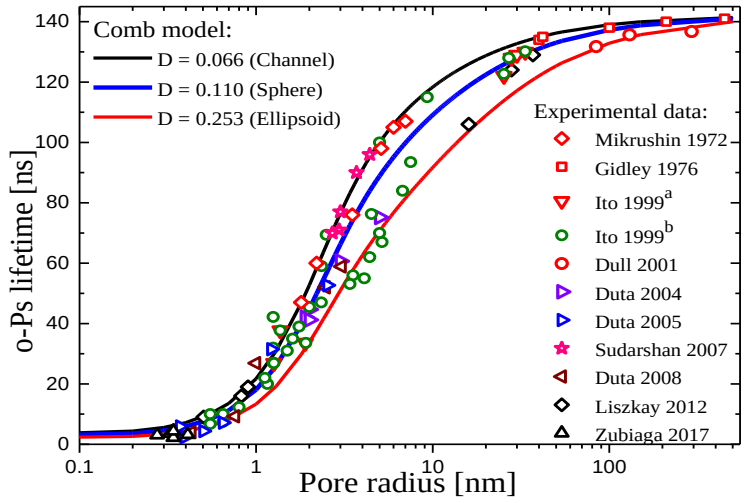

FIG. 5. The Comb model for the different pore geometries and experimental data for porous materials.

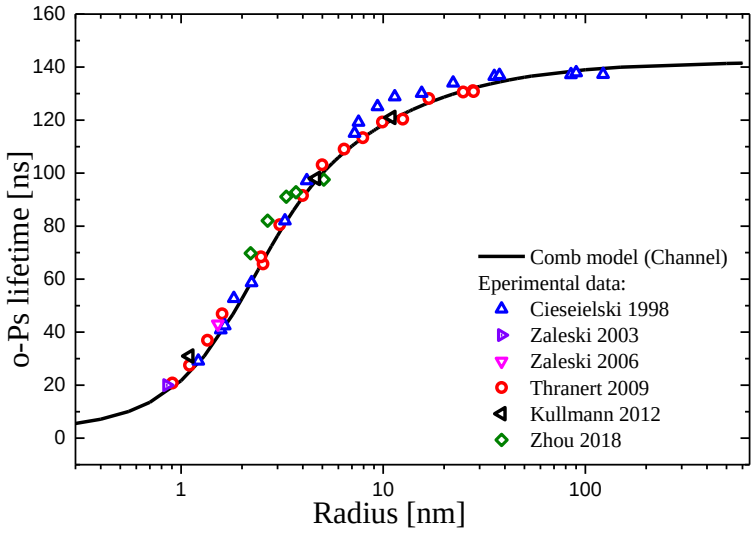

FIG. 6. Verifying the Comb mode for channel pores from experimental data [31, 36].

To verify the Comb model, the experimental o-Ps lifetime of different pore geometries should be used. Unfortunately, the o-Ps lifetime data for the elliptic pores are not available. Hence, we use collected data of the channel pores in Ref. 31 and 36. As indicated in Fig. 6, our model can fit very well the experimental o-Ps lifetimes for the channel pores as the case of the RTE model [31, 32, 36] thereby, confirming the correctness of the model.

Moreover, it is a quite important consequence that the Comb model predicts about the insignificant influence of the different pore geometries on the o-Ps lifetime in the radius range smaller than 0.3 nm (Fig. 5). This can be explained following. As indicated by Dull et al. [10] and Brown el al. [30], the Broglie wavelength of the thermal o-Ps is about 6 nm [10] (1 order of magnitude larger than the pore size) and the effective size of o-Ps is about 0.11 nm [30] (the same order of magnitude of the pore size). Thus, when a thermal o-Ps is localized in the too small pore geometries, its wavelength is bigger than and its effective size is substantial in comparison with the pore size. In this case, the simultaneous effect of the pore volume and the surface is insignificant. This lead to less-differentiated behaviors of o-Ps in the too small pore geometries. Here, we conclude that the Comb model describes well the true nature of positron annihilation physics.

4. CONCLUSSION

In conclusion, we have developed a new model combining the quantum and semi-classical models for calculating the pore size in the extensive range from 0.2 - 400 nm. By considering to the simultaneous effect of pore surface area and the mean free path of o-Ps in the pore, we have proposed the o-Ps diffusion

probabilities for the channel, spherical and elliptic pores which well predicts the o-Ps lifetimes in comparison with experimental data. Consequently, we have found and elucidated for the first time the low lifetimes of o-Ps by forecasting the elliptic geometric. Moreover, in our model, value of $\Delta R = 0.166$ can use for almost porous materials as well as to be simply for calculating free volume size, thereby overcoming the limitation of the previous models.

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NGUỒN GỐC THỜI GIAN SỐNG THẤP CỦA o-Ps ĐỊNH XỨ TRONG CÁC CẤU TRÚC RỖNG LỚN CỦA VẬT LIỆU: PHÁT HIỆN MỚI TỪ MÔ HÌNH KẾT HỢP VẬT LÝ LƯỢNG TỬ VÀ BÁN CỔ ĐIỂN

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Tóm tắt: Hủy positron là phương pháp rất được quan tâm trong ứng dụng nghiên cứu cấu trúc vật liệu ở thang kích thước từ vài Ấ cho đến vài trăm nm. Trong bài báo này, chúng tôi trình bày về một mô hình vật lý mới cho tính toán kích thước lỗ rỗng trong vật liệu xốp từ thời gian sống thực nghiệm của ortho-Positronium (o-Ps) được công bố và cập nhật hơn bốn thập kỷ qua bằng cách kết hợp mô hình vật lý lượng tử và bán cổ điển. Qua việc đề xuất mới thông số xác suất khuếch tán của o-Ps (D) từ lỗ rỗng vào lớp màng electron ảo (ΔR) của vật liệu và xem xét đến hiệu ứng đồng thời của diện tích bề mặt và quãng đường di chuyển tự do trung bình của o-Ps trong lỗ rỗng tới giá trị của D, chúng tôi đã xây dựng thành công mô hình đơn giản cho các cấu hình rỗng bao gồm dạng kênh (channel), cầu (sphere) và elip (ellipsoid). Hơn nữa, lần đầu tiên chúng tôi đã phát hiện và làm sáng tỏ nguồn gốc thời gian sống thấp của o-Ps trong các lỗ rỗng lớn bằng tiên đoán cấu hình elip cho các lỗ rỗng trong vật liệu, điều chưa được hiểu rõ trong hơn hai thập kỷ qua. Điểm nổi bật trong mô hình vật lý của nghiên cứu này so với các công bố trước đó là giá trị ΔR = 0.166 nm có thể sử dụng để tính toán kích thước lỗ rỗng (không phụ thuộc vào quá trình hiệu chuẩn bán thực nghiệm) trong khoảng rộng từ 0.2 – 400 nm cho hầu hết các vật liệu xốp.

Từ khóa: *Positron, thời gian sống o-Ps vật liệu xốp, mô hình vật lý.*