



UNIVERSITEIT VAN PRETORIA
UNIVERSITY OF PRETORIA
YUNIBESITHI YA PRETORIA

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Theoretical calculation of positron states and annihilation rates in BaF_2

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Abstract content (Max 300 words)

Theoretical calculations for electronic structure are a valuable technique in the analysis of positron annihilation experiments. Theoretical calculations predict measured quantities such as annihilation rates and momentum distributions of annihilating electron-positron pair corresponding to vacancy-type defects trapping free positrons. Core electron annihilations are explained using free atom wavefunctions. The enhancement factor, g , was used in the Generalized Gradient Approximation (GGA) to influence both the fluorine and barium electronic annihilation rates. In the GGA, the annihilation rate in fluorine and barium ranges from $0.112 \times 10^{-9} \text{ s}^{-1}$ to $1.580 \times 10^{-9} \text{ s}^{-1}$ ($1s - 2p$) and from $0.011 \times 10^{-9} \text{ s}^{-1}$ to $2.017 \times 10^{-9} \text{ s}^{-1}$ ($1s - 6s$) respectively. Positron lifetimes of delocalized and localized positron in BaF_2 was calculated in the Two-component Density Functional Theory (TCDFT) and found to be 189.60 ps and 203.67 ps respectively. This is a confirmation of vacancy type defect at ambient temperature.

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No

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Yes

Primary author: Mr JILI, Thulani (University of Zululand)

Co-authors: Dr WAMWANGI, Daniel (University of the Witwatersrand); Prof. SIDERAS-HADDAD, Elias (University of the Witwatersrand); Dr TUOMISTO, Filip (Aalto University); Dr NEMRAOUI, Ouassini (University of Zululand)

Presenter: Mr JILI, Thulani (University of Zululand)

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