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Calculation of atomic-based electron-positron annihilation momentum density in superionic barium flouride

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Abstract content
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Theoretical calculations based on the Generalized Gradient Approximation, which takes into account the variation nature of charge density, are performed to retrieve the contributions of atomic core and valence towards positron-electron annihilation momentum density in BaF2. The annihilation momentum of the 6s state electrons with positrons is prominent between 2.5 mrad to 26.8 mrad corresponding to normalized positron-electron annihilation momentum density between 4.6E-2 and 9.0E-5. The 4d dominates the 5p in the momentum range, 3 mrad to 17 mrad. Positron annihilation rates are also calculated within the Independent Particle Model and Generalized Gradient Approximation. Resultant positron-electron annihilation momentum density is compared with experimental results.

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