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Calculation of the contribution of core states in CdF2 to the electron-positron annihilation momentum density using generalized gradient approximation.

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Abstract content
   (Max 300 words)
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Calculations of high momentum components (HMC) in various atomic structures using generalized gradient approximation (GGA) and local density approximation (LDA) have become a prominent tool in positron-electron annihilation momentum density analysis. In the present work we investigate positron-electron annihilation momentum density using GGA. LDA approximation is also employed as a comparison between the two approximations. The probability that 2p electrons in fluorine, with momentum less than 4 mrad, annihilate with positrons is higher than in cadmium. Cadmium 4d electrons dominate the electron-positron annihilation momentum density between 4.3 mrad to well over 40 mrad with 4s electrons dominating in the momentum range between 23.75 mrad and 31.16 mrad. Annihilation rates calculated in the LDA and GGA are found to differ considerably. The difference is discussed at length. The bulk correlation energies for positrons are found to be -9.052 eV (-0.665 Ry) and -8.374 eV (-0.603 Ry) in the LDA and GGA, respectively.

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