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Positron states and annihilation characteristics at the (100), (110), and (111) surfaces of alkali metals

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Abstract

In this paper we present results of theoretical studies of positron states and annihilation characteristics at the clean surfaces of alkali metals. Positron surface states and positron work functions have been computed for the (100), (110), and (111) surfaces of Li, Na, K, Rb, and Cs using the modified superimposed-atom method to account for discrete-lattice effects, and the results are compared with those obtained for the transition-metal surfaces. Stable positron surface states are found in all cases, with the Li states lying about 0.5 eV below the bulk positron band, and other alkali metals having positron surface states a few hundredths of an eV below the bulk bands. The results for the positronium activation energy and positronium work function for the clean surfaces of alkali metals are presented as well. Surface and bulk state lifetimes and probabilities for a positron trapped in a surface state to annihilate with relevant core-level electrons are also computed and compared with available experimental data.