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Asphericity in the Fermi Surface and Fermi Energy of Na-K, Na-Rb and Na-Cs Binary Alloys

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Abstract: Detailed theoretical investigations into asphericity in the Fermi surface (FS) and Fermi energy (FE) of $Na_{1-x}K_x$, $Na_{1-x}Rb_x$, and $Na_{1-x}Cs_x$ binary solid solutions are carried out for the first time. The alloying behavior of the K, Rb, and Cs with the Na generates the Fermi surface distortion (FSD) of bcc simple metals. The FS of Na-K, Na-Rb, and Na-Cs solid solution is a distorted sphere with the largest deviation along [110]. We have found that the impact of local-field correction function on FSD is maximum at [100] point and minimum at [111] point. The exchange and correlation effect is found to suppress the value of FE.

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