

Abstract Submitted
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A multiphase equation of state for Be based on the modified mean-field potential approach SONG HAIFENG, LIU HAIFENG, ZHANG GONGMU, WANG CONG, SUN BO, IAPCM (Institute of Applied Physics and Computational Mathematics), IAPCM TEAM — We present a first-principles scheme to study the multiphase equation of state (EOS) for Be, based on our recently developed modified mean-field potential (MMFP) approach. We first calculate the EOS for Be of hcp and bcc structure, and then compute the melting curve of Be by using MMFP approach. At last, based on the EOS of bcc Be and melting curve and considering the effect of the melting entropy, we obtain the EOS of liquid Be. Based on the results, we obtain the multiphase EOS of Be. The calculated Hugoniot of solid and liquid phase as well as the melting curve are in agreement with available experimental data.

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