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A multiphase equation of state for BeO based on the modified mean-field potential approach HAI-FENG SONG, MING-FENG TIAN, Institute of Applied Physics and Computational Mathematics — We present a first-principles scheme to study the multiphase equation of state (EOS) for BeO, based on the modified mean-field potential (MMFP) approach. We first calculate the EOS for BeO of hexagonal wurtzite and rocksalt structure, and then compute the melting curve of BeO by using MMFP approach. At last, based on the EOS of hexagonal wurtzite BeO and melting curve and considing the effcet of the melting entropy, we obtain the EOS of liquid BeO. Based on the results, we obtain the multiphase EOS of BeO and a phase diagram. The calcutlated Hugoiot is in agreement with available experimental data.

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