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Atomic structure of PdNiP bulk metallic glass from ab initio simulations VIJAY KUMAR, Dr. Vijay Kumar Foundation, Gurgaon, India, T. FUJITA, M.W. CHEN, WPI-AIMR, Tohoku Univ. Sendai, Japan, A. INOUE, Tohoku Univ., Sendai, Japan, Y. KAWAZOE, IMR, Tohoku Univ. Sendai, Japan — The atomic structure of Pd40Ni40P20 bulk metallic glass (BMG) has been simulated using *ab initio* molecular dynamics plane wave method and PAW pseudopotentials. We use generalized gradient approximation to calculate the exchange-correlation energy and a cubic simulation box whose size and shape have been optimized after the BMG has been formed in simulations. The resulting radial distribution function and density agree remarkably well with the experimental data. The structure is analysed in terms of local clusters centered around Pd, Ni and P atoms and their electronic structures have been used to understand the bonding, stability, and the formation of the PdNiP BMG.

Vijay Kumar
Dr. Vijay Kumar Foundation, Gurgaon, India

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