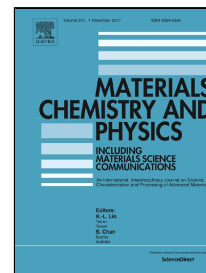


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Structural, elastic and anisotropic properties of CuZr from first-principles calculations

Guohui Yi, Xinyu Zhang, Jinliang Ning, Jiaqian Qin, Xiaowei Sun, Qin Jing, Mingzhen Ma, Riping Liu



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Highlights

1. We systematically investigate structural and elastic properties of CuZr.
2. B19' CuZr shifts to a B33 phase upon geometry optimization.
3. We present detailed anisotropic elastic moduli of the two phases by 3D models.

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