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Structural stability, elastic constants, bonding characteristics and thermal properties of zincblende, rocksalt and fluorite phases in copper nitrides: plane-wave pseudo-potential *ab initio* calculations

Research Article

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Abstract: We report plane-wave pseudo-potential *ab initio* calculations using density functional theory in order to investigate the structural parameters, elastic constants, bonding properties and polycrystalline parameters of copper nitrides in zincblende, rocksalt and fluorite structures. Total and partial densities of states indicate a metallic character of these copper nitrides. We estimate bond strengths and types of atomic bonds using Mulliken charge density population analysis and by calculating the electronic localized function. These results reveal the coexistence of covalent, ionic, and metallic bonding.

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Keywords: nitrides • electronic and bonding properties • elastic constants • electronic localized function

1. Introduction

Transition metal nitrides attract considerable interest for their properties and potential technical applications [1–4]. Both theoretical and experimental effort has gone into studying the early transition metal nitrides [5–12]. The 4*d* and 5*d* series of late transition metals Ru, Rh, Pd, Ag, Os, Ir, Pt, and Au, also known as noble metals, are generally considered not to form nitrides [1], although Cu_3N and Cu_3MN have been reported [13, 14]. Despite the wide interest in making ever better nitrides for applications, the noble metal nitrides have evaded discovery until the recent synthesis of gold [15], and platinum nitrides. In fact, the recent highest pressure of a new material, PtN, was synthesized and recovered in zincblende structure back to

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