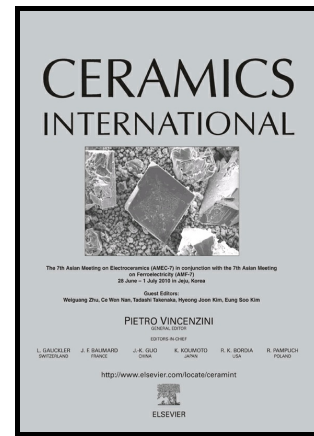


# Author's Accepted Manuscript

Pressure dependent mechanical properties of calcium carbides

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## Pressure dependent mechanical properties of calcium carbides

Hong Jiang<sup>1</sup>, Wei Dong<sup>1</sup>, Xiao-Xue Qu<sup>1</sup>, Kuan Cao<sup>1</sup>, Yue-Hua Su<sup>1</sup>, and Chao Zhang<sup>1\*</sup>

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The mechanical properties of newly synthesized  $\text{Ca}_2\text{C}_3$  and  $\text{Ca}_2\text{C}$  under pressure have been studied by using the first-principles calculations with generalized gradient approximation. The equilibrium geometry, elastic stiffness constants, various moduli, and Pugh's ratio of the  $C2/m$  phase of  $\text{Ca}_2\text{C}_3$  and the  $C2/m$  and  $Pnma$  phases of  $\text{CaC}_2$  are systematically studied. The elastic stiffness constants of  $C2/m$ - $\text{Ca}_2\text{C}_3$  under 0 GPa to 30 GPa,  $C2/m$ - $\text{Ca}_2\text{C}$  under 0 GPa to 7.5 GPa, and  $Pnma$ - $\text{Ca}_2\text{C}$  under 7.5 GPa to 30 GPa satisfy the Born–Huang mechanical criteria. The three phases of calcium carbides exhibit ductile characteristics. The surface constructions of bulk and Young's moduli illustrate the mechanical anisotropy of  $\text{Ca}_2\text{C}_3$  and  $\text{Ca}_2\text{C}$ . Our results are consistent with previously obtained experimental and theoretical data and have significant implications for the application of calcium carbides.

Keywords: Carbides; Mechanical properties; Anisotropic Properties; First-principles calculations

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