

TITLE: Ab initio computations of the electronic, mechanical, and thermal properties of ultra high temperature ceramics (UHTC) ZrB₂ and HfB₂

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ABSTRACT BODY: Refractory materials such as metallic borides, often considered as ultra high temperature ceramics (UHTC), are characterized by high melting point, high hardness, and good chemical inertness. These materials have many applications which require high temperature materials that can operate with no or limited oxidation. Ab initio, first principles methods are the most accurate modeling approaches available and represent a parameter free description of the material based on the quantum mechanical equations. Using these methods, many of the intrinsic properties of these material can be obtained. We performed ab initio calculations based on density functional theory for the UHTC materials ZrB₂ and HfB₂. Computational results are presented for structural information (lattice constants, bond lengths, etc), electronic structure (bonding motifs, densities of states, band structure, etc), thermal quantities (phonon spectra, phonon densities of states, specific heat), as well as information about point defects such as vacancy and antisite formation energies.

KEYWORDS: UHTC, ab initio computation, density functional theory, ZrB₂, HfB₂.