



Multifunctional radiation shielding performance of hafnium-containing MAX-related borides: The impact of a-site chemistry and boron concentration

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ABSTRACT

This study investigates the influence of A-site chemistry and boron concentration on the gamma-ray (γ -ray), neutron, and charged particle attenuation of a series of hafnium-containing MAX-related borides (Hf_2SB , Hf_2SeB , Hf_2InB , Hf_2TeB , Hf_2PbB , Hf_2BiB , Hf_2InB_2 , Hf_2SnB_2 , Hf_3PB_4 , and Hf_3SnB_4) via systematic theoretical calculations. For γ -rays, efficiency is governed by a compositional trade-off between effective atomic number, density, and elemental composition: high atomic number (high-Z) Hf_2BiB and Hf_2PbB exhibited the highest calculated attenuation performance among the investigated MAX-related borides and showed lower half-value layer (HVL) values than pure lead (Pb) at selected photon energies, particularly around 2.5 MeV. Analysis showed that selected light-A-site compositions, particularly Hf_2SB and Hf_3PB_4 , maintain competitive γ -ray attenuation relative to binary HfB_2 by preserving a high hafnium (Hf) fraction, although the relative ranking depends strongly on the photon-energy regime and attenuation parameter considered. For neutrons, performance was primarily driven by boron content. Among the investigated MAX-related borides, the boron-rich Hf_3PB_4 and Hf_3SnB_4 phases demonstrated the highest fast neutron removal cross sections, reaching up to 0.1647 cm^{-1} , and exceeded the B_4C benchmark value used in this study (0.141 cm^{-1}). Notably, these phases also showed short-calculated ranges for protons and alpha particles, suggesting favorable heavy charged-particle stopping behavior associated with their relatively high light-element content. This trade-off identifies Hf_3PB_4 as the most balanced multifunctional candidate among the investigated compositions, combining strong neutron and heavy charged-particle attenuation with competitive γ -ray shielding, and highlights the potential of Hf-containing MAX-related borides for multifunctional radiation-shielding applications.

1. Introduction

The widespread adoption of nuclear technologies in diverse fields, including power generation, medical diagnostics, space exploration, and advanced materials characterization techniques, has driven an increasing demand for effective radiation shielding. While these technologies offer significant societal and technological benefits, they also pose the critical challenge of protecting humans and the environment from harmful ionizing radiation. Designing effective shielding is inherently complex, as different types of radiation, such as gamma-rays (γ -rays), neutrons, and charged particles, interact with matter via distinct mechanisms. Developing effective materials therefore requires carefully tailored properties to address the distinct characteristics of each type of radiation.

High atomic number (high-Z) materials, such as lead (Pb), bismuth (Bi), and tungsten (W), are highly effective at attenuating γ -rays due to their dense electron clouds, which enhance photoelectric absorption and pair production. In contrast, low atomic number (low-Z) materials, such as hydrogen-rich compounds (e.g., water, concrete, and polymers) and boron-containing materials (e.g., B_4C), are particularly effective at

slowing neutrons through elastic scattering, a process in which kinetic energy is efficiently transferred to light nuclei [1-6]. However, this complementary behavior presents a significant challenge, as many applications produce both neutrons and γ -rays simultaneously, necessitating the development of multifunctional shielding materials.

These requirements are particularly pronounced across several key sectors. In the nuclear power industry, reactors generate intense fluxes of both γ -rays and neutrons, demanding that the reactor vessel and biological shield attenuate both to ensure safety [7-11]. Future fusion systems, such as ITER, will also produce high-energy neutrons and γ -rays, necessitating multifunctional shielding to protect both equipment and personnel [12]. Similarly, nuclear waste management and spent fuel transport require materials capable of effectively attenuating mixed-radiation fields [13,14]. In the medical field, therapies like Boron Neutron Capture Therapy (BNCT) intentionally combine thermal neutrons with secondary γ -rays, requiring specialized shielding that precisely targets tumors while sparing healthy tissues [15].

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For space exploration, cosmic rays and reactor systems on nuclear-propelled spacecraft generate complex mixed-radiation fields consisting of high-energy neutrons, γ -rays, and secondary particles, all of which must be mitigated by multifunctional shielding materials [16]. Moreover, neutron capture can itself produce secondary γ -rays, meaning that a shield designed solely for neutron absorption may inadvertently create an additional γ -ray hazard [7]. Addressing this often necessitates complex, multi-layered systems that combine low-Z and high-Z materials, increasing both thickness and weight while complicating design.

To overcome these limitations and simplify shielding designs, recent research has focused on alternative strategies, particularly multifunctional materials capable of simultaneously attenuating multiple radiation types. One established approach involves polymer matrix composites, where the hydrogen-rich polymer moderates neutrons and embedded high-Z particles provide γ -ray attenuation [17-19]. Other promising strategies include high-Z-containing glasses and metallic alloys, where the shielding elements are integrated into the atomic or microstructural framework, enabling effective γ -ray attenuation while maintaining mechanical integrity [20,21]. On the other hand, a particularly promising direction is the synthesis of compound materials that inherently merge complementary shielding properties. In this respect, transition metal borides exemplify this approach, merging high-Z transition metals with low-Z boron to yield inherent multifunctional capabilities. Indeed, previous studies have demonstrated that these borides exhibit excellent γ -ray and neutron radiation shielding performance. For instance, ReB_2 , WB_2 , and TaB_2 show higher γ -ray attenuation than Pb at certain energies, while SmB_6 and DyB_6 provide superior thermal and fast neutron absorption compared with conventional shielding materials like B_4C [2].

Of further note, beyond elemental composition, shielding performance is directly proportional to material density, as a greater number of atoms per unit volume increases the probability of radiation interactions [22]. This density is governed by both the atomic masses of the constituent elements and their crystallographic packing. Therefore, this study focuses on a material family with dense layered atomic arrangements, namely MAX and MAX-related borides.

MAX phases, named after their general chemical formula $\text{M}_{n+1}\text{AX}_n$, are a family of layered hexagonal compounds in which M is typically an early transition metal, A is an A-group element, and X is carbon or nitrogen [23]. Recently, this family has expanded to include boride analogues, such as Zr_2SB , Nb_2SB , and Hf_2SB , where boron occupies the X-site [24,25]. In addition, boron-based MAX-related layered compounds with different stoichiometries have also been reported. For example, M_2AX_2 -type borides such as Ti_2InB_2 and Hf_2InB_2 have been theoretically predicted and subsequently synthesized [26,27], while

boron-rich Hf_3AB_4 -type compounds such as Hf_3PB_4 and Hf_3SnB_4 have been theoretically predicted as MAX-related layered borides [37]. These developments represent structural and compositional extensions of the conventional MAX phase family. MAX and MAX-related phases are attractive due to their unique combination of metallic and ceramic-like properties, including high electrical conductivity, thermal shock tolerance, and radiation damage resistance [28-30].

Within this broad family, hafnium (Hf)-containing MAX-related borides are particularly noteworthy because they offer a wide compositional space for tuning Hf content, A-site chemistry, boron concentration, and density. Hf ($Z=72$) is a high-Z element, making it inherently effective for γ -ray attenuation. Moreover, several of its naturally abundant isotopes, most notably ^{177}Hf and ^{179}Hf , exhibit exceptionally large neutron capture cross sections, enabling efficient thermal neutron absorption [31]. When combined with boron's strong (n, α) absorption, particularly from the ^{10}B isotope [32], these borides are expected to provide a synergistic dual mechanism, simultaneously enhancing γ -ray and thermal neutron shielding.

Despite these promising features, the radiation shielding performance of Hf-containing MAX-related borides remains unexplored. This study addresses this gap by providing a systematic theoretical evaluation of their γ -ray, neutron, and charged-particle attenuation properties. In particular, this work clarifies how A-site chemistry, boron concentration, Hf fraction, and density jointly govern the trade-off between photon, neutron, and charged-particle shielding performance within a single Hf-containing boride family. These results indicate that Hf-containing MAX-related borides can provide multifunctional shielding characteristics through the combined effects of crystal chemistry, high density, Hf content, and tunable boron concentration. Selected compositions show calculated γ -ray attenuation comparable to or better than Pb at specific photon energies and fast neutron removal cross sections higher than the B_4C benchmark value considered in this study. Overall, the study highlights the importance of balancing elemental composition, density, and boron content to address mixed-radiation shielding requirements, positioning Hf-containing MAX-related borides as promising candidates for further investigation.

2. Methodology

Ten Hf-containing MAX-related borides, namely Hf_2SB , Hf_2SeB , Hf_2InB , Hf_2TeB , Hf_2PbB , Hf_2BiB , Hf_2InB_2 , Hf_2SnB_2 , Hf_3PB_4 , and Hf_3SnB_4 , were selected based on prior theoretical and/or experimental studies reporting their structural stability, thermodynamic formability, or synthesis feasibility. Conventional hafnium diboride (HfB_2) was also included as a reference binary boride. Among the investigated compounds, Hf_2SB , Hf_2SeB , Hf_2TeB , and Hf_2InB_2 have been experimentally reported, whereas Hf_2InB , Hf_2BiB , Hf_2SnB_2 , Hf_3PB_4 , Hf_2PbB and

Hf₃SnB₄ are based on theoretical predictions reported in the literature [24,27,33,34]. The density values used in the radiation-shielding calculations were calculated from the reported lattice parameters, unit-cell volumes, formula weights, and crystallographic information of the corresponding compounds and are provided in Table 1.

Table 1. Physical properties of Hf-containing MAX-related borides

Compound	Space group	Lattice parameter a (Å)	Lattice parameter c (Å)	Density (g/cm ³)	Ref.
Hf ₂ SB	P6 ₃ /mmc (194)	3.467	12.105	10.50	[24]
Hf ₂ SeB	P6 ₃ /mmc (194)	3.523	12.478	11.07	[33]
Hf ₂ InB	P6 ₃ /mmc (194)	3.414	15.215	10.44	[35]
Hf ₂ PbB	P6 ₃ /mmc (194)	3.493	14.899	12.15	[36]
Hf ₂ BiB	P6 ₃ /mmc (194)	3.530	14.374	12.34	[36]
Hf ₂ TeB	P6 ₃ /mmc (194)	3.605	13.127	10.87	[34]
Hf ₂ InB ₂	P6̄m2 (187)	3.195	8.319	11.10	[27]
Hf ₂ SnB ₂	P6̄m2 (187)	3.221	8.204	11.12	[37]
Hf ₃ PB ₄	P6̄m2 (187)	3.228	10.459	10.73	[37]
Hf ₃ SnB ₄	P6̄m2 (187)	3.179	11.787	11.21	[37]

The results obtained for the MAX-related borides were systematically compared with those of conventional HfB₂, which has a density of 10.5 g/cm³. γ-ray attenuation was evaluated using the mass attenuation coefficient (MAC, μ_m) and linear attenuation coefficient (LAC, μ), calculated according to the Beer-Lambert attenuation law (Eq. 1-3) and photon interaction data tabulated in the National Institute of Standards and Technology (NIST)/XCOM database where w_i is the weight fraction of element *i* and (μ/ρ)_i is the MAC of the pure element [38,39].

$$I = I_0 e^{-\mu x} \quad (1)$$

$$\mu_m = \frac{\mu}{\rho} = \frac{1}{\rho t} \ln \frac{I_0}{I} \quad (2)$$

$$\mu_m = \sum_i w_i \left(\frac{\mu}{\rho} \right)_i \quad (3)$$

HVL and mean free path (MFP) were determined according to Eq. 4, 5 from the standard attenuation relations [38,39].

$$\text{HVL} = \frac{\ln 2}{\mu} \quad (4)$$

$$\text{MFP} = \frac{1}{\mu} \quad (5)$$

The effective atomic number (Z_{eff}) was obtained from the ratio of the atomic and electronic cross sections using the commonly applied cross-section method given in Eq. 6 [39,41,42]. Atomic cross-section σ_a and electronic cross-section σ_e are determined according to Eq. 6-8, where, A_i and Z_i are the atomic weight and number of element *i*, and f_i is its mole fraction.

$$Z_{\text{eff}} = \frac{\sigma_a}{\sigma_e} \quad (6)$$

$$\sigma_a = \frac{N_A}{A} \mu_m \quad (7)$$

$$\sigma_e = \frac{1}{N_A} \sum_i \frac{f_i A_i}{Z_i} (\mu/\rho)_i \quad (8)$$

Fast neutron attenuation was evaluated using the fast neutron removal cross section (FNRCs, Σ_R), calculated by the conventional mixture-rule approach for compound shielding materials (Eq. 9), where ρ_i is the partial density of element *i* and (Σ_{R/ρ})_i is the mass removal cross-section [39,43-45].

$$\Sigma_R = \sum_i \rho_i \left(\frac{\Sigma_R}{\rho} \right)_i \quad (9)$$

Thermal neutron shielding was assessed using the macroscopic absorption cross section, expressed here as the thermal-neutron linear attenuation coefficient (Σ_a), calculated from elemental microscopic absorption cross-section data reported by Sears (Eq. 10), where M_m is the molar mass (g/mol), n_j is the number of atoms of element *j* per formula unit, and σ_(a,j) is the microscopic absorption cross-section of element *j* (barns) [46].

$$\Sigma_a = \frac{\rho N_A}{M_m} \sum_j n_j \sigma_{a,j} \times 10^{-24} \quad (10)$$

All γ-ray shielding parameters, including MAC, LAC, Z_{eff}, HVL, and MFP, as well as FNRCs, were calculated using the Phy-X/PSD software [38]. Penetration depths, expressed as projected ranges, for protons (H⁺) and alpha particles (He²⁺) were determined using the SRIM Monte Carlo package over the kinetic energy range of 0.1-10 MeV [47], whereas electron range values over the same energy range were obtained from the ESTAR database developed by the NIST [48]. Thermal neutron calculations were performed assuming natural isotopic abundances and monoenergetic thermal neutrons with an incident energy of 25.3 meV [46]. These calculations do not include resonance absorption effects, neutron self-shielding, multiple scattering, moderation history, or geometry-dependent neutron transport effects. Therefore, the obtained thermal neutron LAC values should be interpreted as first-order comparative macroscopic absorption coefficients rather than full neutron transport simulation results.

3. Results and Discussion

The Z_{eff} is a critical descriptor of photon attenuation, reflecting how the weighted electron density of a compound governs its interaction probability with γ-rays. Figure 1a shows the variation of Z_{eff} with photon energy for the studied Hf-containing MAX-related borides, along with the conventional binary boride HfB₂ as a reference. The curves display the characteristic regimes of photon-matter interaction, with photoelectric absorption dominating below ~0.15 MeV, Compton scattering at intermediate energies, and pair production at >5 MeV.

This regime sequence is corroborated by the scattering analysis in Figure 1b. The ratio of incoherent to total scattering (R_{incoherent/total}) for all phases rises steeply above ~0.1 MeV, peaks broadly around 3 MeV, and then gradually declines toward higher energies. This behavior reflects the onset of pair production

beyond several MeV, which increasingly competes with Compton scattering. Nevertheless, incoherent scattering remains the dominant mechanism throughout the ~0.1-5 MeV range, an important window for γ -ray shielding. Within this general trend, however, clear compositional differences emerge, reflecting the balance between A-site element substitution and Hf content in dictating electron density and thereby Z_{eff} .

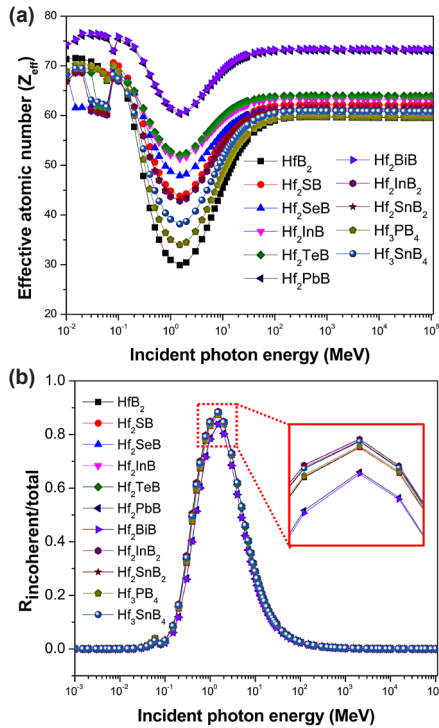


Figure 1. (a) Variation of the effective atomic number and (b) the ratio of incoherent to total scattering ($R_{\text{incoherent/total}}$) as a function of incident photon energy for the Hf-containing MAX-related borides, including Hf_2SB , Hf_2SeB , Hf_2InB , Hf_2TeB , Hf_2PbB , Hf_2BiB , Hf_2InB_2 , Hf_2SnB_2 , Hf_3PB_4 , and Hf_3SnB_4 , together with the conventional binary boride HfB_2 .

At 0.1 MeV, where photoelectric absorption dominates and its cross section approximately scales with the fourth to fifth power of atomic number (Z^{4-5}), therefore heavy atoms are strongly favored [49]. Indeed, Hf_2BiB ($Z_{\text{eff}}=75.93$) and Hf_2PbB ($Z_{\text{eff}}=75.44$) exhibit the highest values. Despite their relatively low Hf fractions (≈ 62 wt%) (Table 2), the presence of the very heavy A-site elements Bi ($Z=83$) and Pb ($Z=82$) more than compensates for the Hf dilution, giving these phases a distinct advantage over other MAX-related borides and binary HfB_2 .

Importantly, several MAX phases with lighter A-site atoms also exceed HfB_2 in Z_{eff} at 0.1 MeV. For instance, Hf_2SB (69.99), Hf_2SeB (68.62), and Hf_3PB_4 (68.84) record higher values despite containing relatively light A-site elements (S, $Z=16$; Se, $Z=34$; P, $Z=15$). This behavior can be rationalized by their Hf weight fractions, which remain close to that of HfB_2 (89.2 wt%). Indeed, Hf_2SB (89.3 wt% Hf) and Hf_3PB_4 (87.5 wt% Hf) retain nearly identical Hf fractions, so even the modest electron density advantage of sulfur or phosphorus relative to boron ($Z=5$) is sufficient to

raise Z_{eff} . In contrast, Hf_2SeB has a more noticeable reduction in Hf content (79.9 wt%), but the higher atomic number of selenium ($Z=34$) offsets this dilution, allowing Z_{eff} to still surpass that of HfB_2 . Thus, light A-site MAX-related phases can achieve higher Z_{eff} than HfB_2 through the combined effect of preserved Hf content and the modest but meaningful contribution of their A-site atoms.

Table 2. Weight fractions of constituent elements and Z_{eff} at 0.1, 1.5, and 10 MeV for Hf-containing MAX-related borides and HfB_2 .

Compound	Hafnium wt. %	A-site wt. %	Boron wt. %	Z_{eff} 0.1 MeV	Z_{eff} 1.5 MeV	Z_{eff} 10 MeV
HfB_2	89.2	-	10.8	68.30	29.90	45.50
Hf_2SB	89.3	8.0	2.7	69.99	43.80	55.07
Hf_2SeB	79.9	17.7	2.4	68.62	47.88	56.43
Hf_2InB	74.0	23.8	2.2	67.67	51.35	59.14
Hf_2TeB	72.1	25.8	2.2	67.71	52.07	59.83
Hf_2PbB	62.1	36.0	1.9	75.44	60.30	68.75
Hf_2BiB	61.9	36.3	1.9	75.93	60.63	69.10
Hf_2InB_2	72.4	23.3	4.4	66.91	42.81	53.99
Hf_2SnB_2	71.9	23.9	4.4	66.92	43.01	54.21
Hf_3PB_4	87.5	5.1	7.1	68.84	33.97	48.27
Hf_3SnB_4	81.3	18.0	6.6	67.34	38.16	51.39

Counterintuitively, MAX phases containing intermediate-Z A-site atoms such as In ($Z=49$), Sn ($Z=50$), or Te ($Z=52$) show noticeably lower Z_{eff} than both HfB_2 and the lighter A-site phases. This outcome arises because incorporating these heavier A-site atoms substantially reduces the Hf weight fraction (≈ 72 -74 wt%), diluting the dominant high-Z contribution of Hf. Although In, Sn, and Te are significantly heavier than S, Se, or P, their gain in atomic number is not sufficient to offset the larger reduction in Hf content. As a result, their overall electron density, and hence Z_{eff} , falls behind that of HfB_2 and the light MAX-related phases in the low-energy photoelectric regime. This trend highlights that lighter A-site incorporation does not necessarily weaken photon attenuation capacity against low energy photons, and in certain cases can be more favorable than intermediate-Z substitutions.

At 1.5 MeV, all compounds exhibit their minimum Z_{eff} values, marking the dominance of the Compton scattering regime, where Z_{eff} primarily scales with the material's electron density per unit mass (effective Z/A ratio) [49]. A notable trend shift in compound ranking is observed compared to the 0.1 MeV data. Indeed, at 1.5 MeV, all MAX-related borides recorded Z_{eff} values higher than HfB_2 . While Hf_2BiB (60.63) and Hf_2PbB (60.30) maintain the highest Z_{eff} , the MAX phases are now ordered based on the absolute electron contribution of the A-site element, overriding the low-energy preference for high Hf content. Specifically, MAX-related borides with intermediate-Z A-site elements (In, Sn, Te) now generally outperform those with lighter A-site elements (S, Se, P).

For instance, Hf_2TeB (52.07) and Hf_2InB (51.35) rank above Hf_2SeB (47.88) and Hf_2SB (43.80). Although the intermediate-Z atoms cause greater dilution of the Hf weight fraction, their inherently larger atomic number contributes a proportionally higher number of electrons to the overall material, which dictates the higher effective Z/A ratio and, thus, the Z_{eff} at this energy.

On the other hand, at 1.5 MeV, the lowest Z_{eff} value is recorded by HfB_2 (29.90). Despite having the high Hf weight fraction (≈ 89.2 wt%), the compound contains a substantial B component ($Z=5$), whose presence significantly lowers the material's overall effective Z/A ratio relative to the MAX phases. This observation highlights the minor role of Hf content preservation when the electron density becomes the dominant attenuation mechanism.

At 10 MeV, Z_{eff} increases due to the Z^2 scaling of the pair production cross-section [49,50]. Heavy A-site atoms again dominate. Indeed, Hf_2BiB (69.10) and Hf_2PbB (68.75) retain the highest values. The overall ranking established in the Compton regime largely persists here. MAX phases with intermediate-Z A-site elements (Te, In) form the next tier (Hf_2TeB , 59.83; Hf_2InB , 59.14), followed by those incorporating lighter A-site elements (S, Se) (Hf_2SeB , 56.43; Hf_2SB , 55.07). The remaining Hf_2AB_2 and Hf_3AB_4 phases with relatively higher boron content occupy the lower intermediate range: Hf_2SnB_2 (54.21), Hf_2InB_2 (53.99), Hf_3SnB_4 (51.39), and Hf_3PB_4 (48.27). HfB_2 (45.50) again remains the lowest, consistent with its limited total electron content. The persistence of this order confirms that at high energies, Z_{eff} is more sensitive to the absolute electron contribution of heavy atoms than to the Hf fraction, suggesting improved calculated photon attenuation performance for Bi- and Pb-containing phases under these conditions.

The corresponding MAC values (Figure S1, Table S1) are in line with the Z_{eff} -derived trends. Nevertheless, distinct abrupt increases in MAC are observed in the low-energy region, which correspond to the K-absorption edges of the constituent elements.

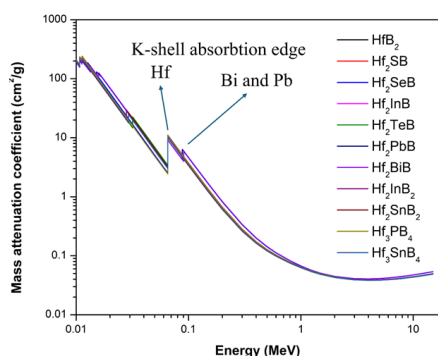


Figure S1. Variation of the mass attenuation coefficient (MAC) with the incident photon energy for the Hf-containing MAX phase borides, including Hf_2SB , Hf_2SeB , Hf_2InB , Hf_2TeB , Hf_2PbB , Hf_2BiB , Hf_2InB_2 , Hf_2SnB_2 , Hf_3PB_4 , and Hf_3SnB_4 , along with the conventional binary boride HfB_2 .

These increases occur when the incident photon energy matches the binding energy of inner-shell (K-shell)

electrons, causing a sudden surge in photoelectric absorption. For instance, a prominent K-edge is visible for Hf around 65.35 keV. Heavier elements, such as Pb and Bi, also contribute absorption edges at higher energies, around 88.0 keV and 90.52 keV,[51] respectively, as depicted in Figure S1.

Besides, at 0.1 MeV, the photoelectric-dominated regime strongly favors very heavy A-site atoms. Indeed, Hf_2BiB (4.652 cm^2/g) and Hf_2PbB (4.580 cm^2/g) show the largest MAC values, corresponding to 25.1% and 23.1% higher attenuation than HfB_2 (3.719 cm^2/g), respectively. Light A-site MAX-related phases also modestly outperform HfB_2 . For example, Hf_2SB (3.727 cm^2/g) exceed HfB_2 by 2-3%, reflecting their preserved Hf fractions (~ 87 -89 wt%) and the small but non-negligible contribution of S relative to B. Hf_2SeB (3.433 cm^2/g) and Hf_2InB (3.458 cm^2/g), by contrast, fall ~ 7 -8% below HfB_2 , as the reduction in Hf fraction (72-80 wt%) outweighs the modest benefit of their higher-Z A-site atoms. The lowest MAC among the series is observed for Hf_2InB_2 (3.385 cm^2/g) and Hf_2SnB_2 (3.387 cm^2/g), which are $\sim 9\%$ below HfB_2 due to both Hf dilution and additional boron content.

In the intermediate energy range, where Compton scattering dominates, the MAC values reach their absolute minimum at 3-4 MeV (and remain nearly constant up to 6 MeV), converging tightly across the series to ≈ 0.038 -0.041 cm^2/g . High-Z Bi/Pb phases still preserve the modest residual advantage. Indeed, Hf_2BiB (0.041 cm^2/g) and Hf_2PbB (0.040 cm^2/g) remain about 5% higher than HfB_2 (0.039 cm^2/g), marking a pronounced reduction in compositional contrast from the $\sim 25\%$ enhancement observed in the low-energy photoelectric region.

At higher energies, where pair production becomes important, the sensitivity to high-Z atoms increases again; Bi- and Pb-containing phases continue to show higher MAC than HfB_2 (Table S1), but the absolute inter-material differences are reduced relative to the low-energy photoelectric regime. For example, at 10 MeV, MAC values remain tightly grouped between 0.043-0.047 cm^2/g . Hf_2BiB (0.047 cm^2/g) and Hf_2PbB (0.047 cm^2/g) sustain a $\sim 7\%$ advantage over HfB_2 (0.044 cm^2/g). All other phases are essentially indistinguishable from HfB_2 , with deviations of $\leq 2\%$. This convergence highlights that at very high energies, MAC is largely governed by bulk electron content, minimizing the influence of compositional differences apart from the heaviest elements.

While the MAC and Z_{eff} describe the intrinsic photon-matter interaction probabilities dictated by atomic composition, practical shielding performance depends on bulk material properties, particularly density. Incorporating density into the LAC allows a direct evaluation of macroscopic γ -ray attenuation, while the HVL and MFP translate this information into concrete shielding thicknesses and photon travel distances (Table S2-4).

Table S1. MAC of the hafnium-containing MAX phase borides across the energy range 1 keV to 100 GeV.

Energy (MeV)	Hf ₂ SB	Hf ₂ SeB	Hf ₂ InB	Hf ₂ TeB	Hf ₂ PbB	Hf ₂ BiB	Hf ₂ InB ₂	Hf ₂ SnB ₂	Hf ₃ PB ₄	Hf ₃ SnB ₄
1.00E-03	3205.849	3104.527	4352.115	4602.344	3971.072	4059.156	4283.676	4394.359	3113.755	4025.213
1.50E-03	1406.520	2142.048	1854.790	2010.534	1780.715	1822.821	1822.404	1872.037	1367.831	1727.679
2.00E-03	3246.187	3425.408	3039.383	3067.163	2699.139	2717.312	2976.289	2986.121	3185.488	3054.746
3.00E-03	1687.302	1611.401	1447.281	1450.218	1806.768	1839.273	1416.594	1417.912	1613.160	1465.077
4.00E-03	842.111	801.042	948.380	723.613	1001.115	1018.247	928.023	860.871	805.913	841.144
5.00E-03	484.763	460.045	572.011	600.908	580.898	591.284	559.690	569.647	464.348	537.373
6.00E-03	306.762	290.712	360.767	381.233	369.880	376.841	352.984	359.456	294.102	339.520
8.00E-03	147.887	139.910	173.110	182.834	179.968	183.444	169.368	172.545	142.014	163.310
1.00E-02	209.501	191.713	201.683	204.523	189.973	191.729	197.292	198.281	204.250	200.322
1.50E-02	116.381	121.303	105.971	106.012	120.274	121.837	103.659	103.719	113.918	106.976
2.00E-02	54.891	57.164	49.896	49.901	68.923	70.114	48.809	48.831	53.756	50.408
3.00E-02	18.907	19.592	24.919	17.154	23.956	24.409	24.377	24.908	18.529	23.138
4.00E-02	8.857	9.126	11.728	12.403	11.279	11.503	11.475	11.699	8.685	10.863
5.00E-02	4.942	5.065	6.507	6.901	6.302	6.430	6.369	6.494	4.848	6.038
6.00E-02	3.090	3.150	4.034	4.281	3.935	4.016	3.949	4.029	3.033	3.753
8.00E-02	6.587	6.070	6.132	6.138	5.438	5.466	6.001	6.006	6.478	6.168
1.00E-01	3.727	3.433	3.458	3.459	4.580	4.652	3.385	3.387	3.667	3.482
1.50E-01	1.334	1.231	1.235	1.234	1.645	1.671	1.211	1.211	1.313	1.246
2.00E-01	0.669	0.620	0.621	0.620	0.818	0.831	0.610	0.609	0.659	0.626
3.00E-01	0.284	0.267	0.267	0.266	0.337	0.342	0.263	0.263	0.281	0.269
4.00E-01	0.174	0.165	0.165	0.164	0.199	0.202	0.163	0.163	0.172	0.166
5.00E-01	0.127	0.122	0.122	0.121	0.142	0.143	0.121	0.121	0.126	0.123
6.00E-01	0.103	0.099	0.099	0.099	0.112	0.113	0.099	0.099	0.102	0.100
8.00E-01	0.078	0.076	0.076	0.075	0.082	0.083	0.075	0.075	0.077	0.076
1.00E+00	0.065	0.063	0.063	0.063	0.067	0.067	0.063	0.063	0.064	0.063
1.50E+00	0.050	0.049	0.049	0.048	0.050	0.051	0.049	0.049	0.049	0.049
2.00E+00	0.044	0.043	0.043	0.043	0.045	0.045	0.043	0.043	0.044	0.043
3.00E+00	0.040	0.039	0.039	0.039	0.041	0.041	0.039	0.039	0.040	0.039
4.00E+00	0.039	0.038	0.039	0.038	0.040	0.041	0.038	0.038	0.039	0.038
5.00E+00	0.039	0.039	0.039	0.039	0.041	0.041	0.039	0.039	0.039	0.039
6.00E+00	0.040	0.039	0.040	0.040	0.042	0.042	0.039	0.039	0.039	0.039
7.00E+00	0.041	0.040	0.041	0.041	0.043	0.043	0.040	0.040	0.040	0.040
8.00E+00	0.042	0.041	0.042	0.042	0.045	0.045	0.041	0.041	0.041	0.041
9.00E+00	0.043	0.042	0.043	0.043	0.046	0.046	0.043	0.043	0.042	0.043
1.00E+01	0.044	0.043	0.044	0.044	0.047	0.047	0.044	0.044	0.044	0.044
1.10E+01	0.045	0.045	0.045	0.045	0.049	0.049	0.045	0.045	0.045	0.045
1.20E+01	0.047	0.046	0.047	0.046	0.050	0.050	0.046	0.046	0.046	0.046
1.30E+01	0.048	0.047	0.048	0.047	0.051	0.051	0.047	0.047	0.047	0.047
1.40E+01	0.049	0.048	0.049	0.049	0.052	0.053	0.048	0.048	0.048	0.048
1.50E+01	0.050	0.049	0.050	0.050	0.054	0.054	0.049	0.049	0.049	0.049
1.60E+01	0.051	0.050	0.051	0.051	0.055	0.055	0.050	0.050	0.050	0.050
1.80E+01	0.052	0.051	0.053	0.052	0.057	0.057	0.052	0.052	0.051	0.052
2.00E+01	0.054	0.053	0.054	0.054	0.059	0.059	0.053	0.053	0.053	0.053
2.20E+01	0.056	0.055	0.056	0.056	0.060	0.061	0.055	0.055	0.055	0.055
2.40E+01	0.057	0.056	0.057	0.057	0.062	0.062	0.056	0.056	0.056	0.056
2.60E+01	0.058	0.057	0.059	0.058	0.063	0.064	0.058	0.058	0.057	0.057
2.80E+01	0.060	0.058	0.060	0.060	0.065	0.065	0.059	0.059	0.058	0.059
3.00E+01	0.061	0.060	0.061	0.061	0.066	0.066	0.060	0.060	0.060	0.060
4.00E+01	0.066	0.064	0.066	0.066	0.072	0.072	0.065	0.065	0.064	0.065
5.00E+01	0.069	0.068	0.070	0.069	0.076	0.076	0.068	0.068	0.068	0.068
6.00E+01	0.072	0.071	0.073	0.072	0.079	0.079	0.071	0.071	0.071	0.071
8.00E+01	0.077	0.075	0.077	0.077	0.084	0.084	0.076	0.076	0.075	0.075
1.00E+02	0.080	0.078	0.080	0.080	0.087	0.088	0.079	0.079	0.078	0.079
1.50E+02	0.085	0.083	0.085	0.085	0.093	0.093	0.084	0.084	0.083	0.084
2.00E+02	0.088	0.086	0.088	0.088	0.096	0.097	0.087	0.087	0.086	0.087
3.00E+02	0.092	0.090	0.092	0.092	0.100	0.101	0.090	0.090	0.090	0.090
4.00E+02	0.094	0.092	0.094	0.094	0.103	0.103	0.092	0.092	0.092	0.092
5.00E+02	0.095	0.093	0.096	0.095	0.104	0.105	0.094	0.094	0.093	0.094
6.00E+02	0.096	0.094	0.097	0.096	0.105	0.106	0.095	0.095	0.094	0.095
8.00E+02	0.097	0.095	0.098	0.098	0.107	0.107	0.096	0.096	0.095	0.096
1.00E+03	0.098	0.096	0.099	0.098	0.108	0.108	0.097	0.097	0.096	0.097
1.50E+03	0.100	0.097	0.100	0.100	0.109	0.109	0.098	0.098	0.097	0.098
2.00E+03	0.100	0.098	0.101	0.100	0.110	0.110	0.099	0.099	0.098	0.099
3.00E+03	0.101	0.099	0.101	0.101	0.110	0.111	0.099	0.099	0.099	0.099
4.00E+03	0.101	0.099	0.102	0.101	0.111	0.111	0.100	0.100	0.099	0.100
5.00E+03	0.102	0.099	0.102	0.102	0.111	0.112	0.100	0.100	0.099	0.100
6.00E+03	0.102	0.100	0.102	0.102	0.111	0.112	0.100	0.100	0.099	0.100
8.00E+03	0.102	0.100	0.102	0.102	0.112	0.112	0.101	0.100	0.100	0.100
1.00E+04	0.102	0.100	0.103	0.102	0.112	0.112	0.101	0.101	0.100	0.100
1.50E+04	0.102	0.100	0.103	0.102	0.112	0.112	0.101	0.101	0.100	0.101
2.00E+04	0.102	0.100	0.103	0.103	0.112	0.113	0.101	0.101	0.100	0.101
3.00E+04	0.103	0.100	0.103	0.103	0.112	0.113	0.101	0.101	0.100	0.101
4.00E+04	0.103	0.100	0.103	0.103	0.112	0.113	0.101	0.101	0.100	0.101
5.00E+04	0.103	0.100	0.103	0.103	0.112	0.113	0.101	0.101	0.100	0.101
6.00E+04	0.103	0.100	0.103	0.103	0.112	0.113	0.101	0.101	0.100	0.101
8.00E+04	0.103	0.100	0.103	0.103	0.112	0.113	0.101	0.101	0.100	0.101
1.00E+05	0.103	0.101	0.103	0.103	0.112	0.113	0.101	0.101	0.100	0.101

Table S2. Linear attenuation coefficient (LAC) of the hafnium-containing MAX phase borides across the energy range 1 keV to 100 GeV.

Energy (MeV)	Hf ₂ SB	Hf ₂ SeB	Hf ₂ InB	Hf ₂ TeB	Hf ₂ PbB	Hf ₂ BiB	Hf ₂ InB ₂	Hf ₂ SnB ₂	Hf ₃ PB ₄	Hf ₃ SnB ₄
1.00E-03	33789.64	34367.11	45436.01	50027.47	48248.53	50089.98	47548.81	48865.27	33410.59	45122.63
1.50E-03	14824.72	23712.47	19364.01	21854.50	21635.69	22493.67	20228.68	20817.05	14676.83	19367.28
2.00E-03	34214.81	37919.27	31731.16	33340.06	32794.54	33531.63	33036.81	33205.66	34180.28	34243.7
3.00E-03	17784.16	17838.2	15109.69	15763.87	21952.23	22696.63	15724.19	15767.18	17309.2	16423.51
4.00E-03	8875.85	8867.54	9901.07	7865.67	12163.55	12565.17	10301.05	9572.88	8647.44	9429.22
5.00E-03	5109.4	5092.7	5971.79	6531.87	7057.91	7296.44	6212.56	6334.47	4982.45	6023.95
6.00E-03	3233.27	3218.18	3766.41	4144.01	4494.05	4650.22	3918.12	3997.15	3155.71	3806.02
8.00E-03	1558.73	1548.8	1807.27	1987.41	2186.61	2263.7	1879.99	1918.7	1523.81	1830.71
1.00E-02	2208.14	2122.26	2105.57	2223.16	2308.17	2365.94	2189.94	2204.88	2191.60	2245.61
1.50E-02	1226.65	1342.83	1106.33	1152.35	1461.33	1503.47	1150.62	1153.35	1222.34	1199.2
2.00E-02	578.55	632.80	520.91	542.43	837.46	865.21	541.78	543	576.8	565.07
3.00E-02	199.28	216.89	260.15	186.46	291.06	301.21	270.59	276.98	198.82	259.37
4.00E-02	93.355	101.029	122.444	134.823	137.039	141.95	127.376	130.090	93.19	121.77
5.00E-02	52.094	56.066	67.938	75.010	76.572	79.341	70.691	72.210	52.023	67.683
6.00E-02	32.569	34.875	42.112	46.538	47.812	49.554	43.831	44.802	32.541	42.072
8.00E-02	69.427	67.192	64.017	66.724	66.073	67.449	66.608	66.783	69.508	69.146
1.00E-01	39.287	37.999	36.099	37.604	55.653	57.402	37.574	37.666	39.343	39.038
1.50E-01	14.063	13.629	12.896	13.418	19.991	20.621	13.441	13.468	14.093	13.963
2.00E-01	7.047	6.862	6.480	6.735	9.933	10.251	6.766	6.778	7.070	7.017
3.00E-01	2.995	2.952	2.783	2.886	4.092	4.218	2.918	2.921	3.011	3.010
4.00E-01	1.832	1.828	1.722	1.783	2.420	2.490	1.812	1.813	1.846	1.860
5.00E-01	1.343	1.352	1.274	1.318	1.724	1.770	1.345	1.345	1.356	1.375
6.00E-01	1.085	1.100	1.037	1.071	1.361	1.396	1.096	1.096	1.097	1.117
8.00E-01	0.820	0.838	0.790	0.816	0.998	1.021	0.838	0.837	0.830	0.851
1.00E+00	0.682	0.701	0.661	0.682	0.815	0.833	0.702	0.701	0.691	0.711
1.50E+00	0.523	0.539	0.509	0.525	0.613	0.625	0.541	0.541	0.530	0.547
2.00E+00	0.463	0.478	0.452	0.466	0.542	0.553	0.480	0.479	0.468	0.485
3.00E+00	0.420	0.433	0.411	0.424	0.497	0.507	0.436	0.435	0.424	0.440
4.00E+00	0.411	0.424	0.404	0.417	0.491	0.501	0.427	0.426	0.415	0.431
5.00E+00	0.414	0.427	0.407	0.421	0.498	0.508	0.429	0.430	0.417	0.434
6.00E+00	0.422	0.434	0.415	0.430	0.511	0.521	0.437	0.438	0.424	0.442
7.00E+00	0.432	0.445	0.426	0.441	0.526	0.536	0.448	0.448	0.433	0.452
8.00E+00	0.443	0.456	0.438	0.453	0.542	0.553	0.460	0.460	0.444	0.464
9.00E+00	0.455	0.468	0.450	0.466	0.558	0.569	0.472	0.473	0.456	0.476
1.00E+01	0.467	0.481	0.462	0.479	0.575	0.586	0.485	0.485	0.468	0.489
1.10E+01	0.479	0.493	0.474	0.491	0.591	0.603	0.497	0.498	0.479	0.502
1.20E+01	0.491	0.505	0.486	0.504	0.607	0.619	0.510	0.510	0.491	0.514
1.30E+01	0.503	0.517	0.498	0.516	0.622	0.635	0.522	0.522	0.502	0.526
1.40E+01	0.514	0.529	0.509	0.528	0.637	0.650	0.533	0.534	0.513	0.538
1.50E+01	0.524	0.539	0.520	0.539	0.651	0.664	0.544	0.545	0.524	0.549
1.60E+01	0.534	0.550	0.530	0.549	0.542	0.678	0.555	0.555	0.534	0.560
1.80E+01	0.553	0.569	0.549	0.569	0.497	0.703	0.574	0.435	0.552	0.579
2.00E+01	0.571	0.587	0.566	0.587	0.491	0.726	0.592	0.426	0.570	0.597
2.20E+01	0.587	0.603	0.583	0.604	0.498	0.748	0.609	0.430	0.586	0.614
2.40E+01	0.602	0.619	0.598	0.620	0.511	0.768	0.625	0.438	0.600	0.630
2.60E+01	0.616	0.633	0.612	0.634	0.526	0.787	0.639	0.448	0.614	0.645
2.80E+01	0.629	0.646	0.625	0.648	0.542	0.804	0.653	0.460	0.627	0.658
3.00E+01	0.641	0.659	0.637	0.661	0.558	0.820	0.665	0.473	0.639	0.671
4.00E+01	0.692	0.711	0.688	0.713	0.575	0.887	0.718	0.485	0.690	0.724
5.00E+01	0.731	0.752	0.727	0.754	0.591	0.939	0.759	0.498	0.728	0.765
6.00E+01	0.762	0.783	0.758	0.786	0.607	0.980	0.791	0.510	0.759	0.797
8.00E+01	0.809	0.831	0.804	0.834	0.622	1.040	0.839	0.522	0.806	0.846
1.00E+02	0.842	0.866	0.838	0.869	0.637	1.084	0.874	0.534	0.839	0.881
1.50E+02	0.896	0.921	0.891	0.925	0.651	1.153	0.930	0.545	0.892	0.937
2.00E+02	0.928	0.954	0.924	0.958	0.664	1.195	0.963	0.555	0.924	0.971
3.00E+02	0.967	0.993	0.961	0.998	0.689	1.244	1.003	0.575	0.962	1.011
4.00E+02	0.988	1.016	0.983	1.020	0.712	1.273	1.026	0.593	0.984	1.034
5.00E+02	1.003	1.031	0.998	1.035	0.733	1.291	1.041	0.610	0.998	1.049
6.00E+02	1.013	1.041	1.008	1.046	0.753	1.305	1.052	0.625	1.008	1.060
8.00E+02	1.027	1.056	1.022	1.060	0.771	1.322	1.066	0.640	1.022	1.075
1.00E+03	1.036	1.065	1.031	1.070	0.788	1.334	1.075	0.653	1.031	1.084
1.50E+03	1.049	1.078	1.044	1.083	0.804	1.351	1.089	0.666	1.044	1.098
2.00E+03	1.056	1.086	1.051	1.091	0.870	1.360	1.096	0.719	1.051	1.105
3.00E+03	1.064	1.093	1.059	1.098	0.920	1.369	1.104	0.760	1.059	1.113
4.00E+03	1.068	1.098	1.063	1.103	0.960	1.375	1.109	0.792	1.063	1.117
5.00E+03	1.071	1.100	1.065	1.106	1.019	1.378	1.111	0.840	1.066	1.120
6.00E+03	1.073	1.102	1.067	1.108	1.062	1.381	1.113	0.875	1.068	1.122
8.00E+03	1.075	1.105	1.070	1.110	1.130	1.384	1.116	0.931	1.070	1.125
1.00E+04	1.077	1.106	1.071	1.112	1.171	1.386	1.118	0.965	1.071	1.126
1.50E+04	1.078	1.108	1.073	1.114	1.219	1.388	1.120	1.004	1.073	1.128
2.00E+04	1.080	1.110	1.074	1.115	1.247	1.390	1.121	1.027	1.075	1.130
3.00E+04	1.081	1.111	1.075	1.116	1.265	1.391	1.122	1.042	1.076	1.131
4.00E+04	1.081	1.111	1.076	1.117	1.278	1.392	1.123	1.053	1.076	1.132
5.00E+04	1.082	1.112	1.077	1.117	1.296	1.393	1.123	1.068	1.077	1.132
6.00E+04	1.082	1.112	1.077	1.117	1.307	1.393	1.123	1.077	1.077	1.132
8.00E+04	1.082	1.112	1.077	1.118	1.323	1.393	1.124	1.091	1.077	1.132
1.00E+05	1.083	1.113	1.077	1.118	1.332	1.394	1.124	1.098	1.078	1.133

Table S3. Half value layer (HVL, cm) of the hafnium-containing MAX phase borides in the energy range from 1 keV to 100 GeV.										
Energy (MeV)	Hf ₂ SB	Hf ₂ SeB	Hf ₂ InB	Hf ₂ TeB	Hf ₂ PbB	Hf ₂ BiB	Hf ₂ InB ₂	Hf ₂ SnB ₂	Hf ₃ PB ₄	Hf ₃ SnB ₄
1.00E-03	0.00002	0.00002	0.00002	0.00001	0.00001	0.00001	0.00001	0.00001	0.00002	0.00002
1.50E-03	0.00005	0.00003	0.00004	0.00003	0.00003	0.00003	0.00003	0.00003	0.00005	0.00004
2.00E-03	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002
3.00E-03	0.00004	0.00004	0.00005	0.00004	0.00003	0.00003	0.00004	0.00004	0.00004	0.00004
4.00E-03	0.00008	0.00008	0.00007	0.00009	0.00006	0.00006	0.00007	0.00007	0.00008	0.00007
5.00E-03	0.00014	0.00014	0.00012	0.00011	0.00010	0.00009	0.00011	0.00011	0.00014	0.00012
6.00E-03	0.00021	0.00022	0.00018	0.00017	0.00015	0.00015	0.00018	0.00017	0.00022	0.00018
8.00E-03	0.00044	0.00045	0.00038	0.00035	0.00032	0.00031	0.00037	0.00036	0.00045	0.00038
1.00E-02	0.00031	0.00033	0.00033	0.00031	0.00030	0.00029	0.00032	0.00031	0.00032	0.00031
1.50E-02	0.00057	0.00052	0.00063	0.00060	0.00047	0.00046	0.00060	0.00060	0.00057	0.00058
2.00E-02	0.00120	0.00110	0.00133	0.00128	0.00083	0.00080	0.00128	0.00128	0.00120	0.00123
3.00E-02	0.00348	0.00320	0.00266	0.00372	0.00238	0.00230	0.00256	0.00250	0.00349	0.00267
4.00E-02	0.00742	0.00686	0.00566	0.00514	0.00506	0.00488	0.00544	0.00533	0.00744	0.00569
5.00E-02	0.01331	0.01236	0.01020	0.00924	0.00905	0.00874	0.00981	0.00960	0.01332	0.01024
6.00E-02	0.02128	0.01988	0.01646	0.01489	0.01450	0.01399	0.01581	0.01547	0.02130	0.01648
8.00E-02	0.00998	0.01032	0.01083	0.01039	0.01049	0.01028	0.01041	0.01038	0.00997	0.01002
1.00E-01	0.01764	0.01824	0.01920	0.01843	0.01245	0.01208	0.01845	0.01840	0.01762	0.01776
1.50E-01	0.04929	0.05086	0.05375	0.05166	0.03467	0.03361	0.05157	0.05147	0.04918	0.04964
2.00E-01	0.09836	0.10101	0.10697	0.10292	0.06978	0.06762	0.10244	0.10227	0.09804	0.09879
3.00E-01	0.23146	0.23478	0.24908	0.24017	0.16939	0.16434	0.23755	0.23731	0.23019	0.23026
4.00E-01	0.37826	0.37925	0.40248	0.38874	0.28637	0.27835	0.38244	0.38225	0.37540	0.37260
5.00E-01	0.51601	0.51267	0.54397	0.52608	0.40211	0.39153	0.51546	0.51541	0.51128	0.50423
6.00E-01	0.63861	0.63028	0.66862	0.64713	0.50914	0.49644	0.63231	0.63242	0.63201	0.62035
8.00E-01	0.84519	0.82707	0.87697	0.84967	0.69476	0.67890	0.82727	0.82768	0.83520	0.81468
1.00E+00	1.01567	0.98903	1.04841	1.01638	0.85065	0.83236	0.98758	0.98820	1.00275	0.97460
1.50E+00	1.32598	1.28496	1.36089	1.32000	1.13164	1.10910	1.28048	1.28146	1.30826	1.26646
2.00E+00	1.49843	1.45142	1.53508	1.48854	1.27879	1.25364	1.44539	1.44637	1.47951	1.43021
3.00E+00	1.65045	1.59977	1.68583	1.63318	1.39501	1.36787	1.59139	1.59193	1.63344	1.57524
4.00E+00	1.68566	1.63515	1.71744	1.66236	1.41141	1.38402	1.62515	1.62523	1.67208	1.60913
5.00E+00	1.67437	1.62499	1.70220	1.64644	1.39095	1.36392	1.61390	1.61362	1.66398	1.59846
6.00E+00	1.64387	1.59598	1.66848	1.61298	1.35697	1.33056	1.58437	1.58383	1.63616	1.56959
7.00E+00	1.60537	1.55882	1.62708	1.57234	1.31855	1.29267	1.54697	1.54619	1.59976	1.53285
8.00E+00	1.56433	1.51923	1.58365	1.52984	1.27958	1.25452	1.50719	1.50626	1.56039	1.49370
9.00E+00	1.52345	1.47968	1.54075	1.48805	1.24199	1.21756	1.46756	1.46657	1.52083	1.45469
1.00E+01	1.48415	1.44169	1.49983	1.44818	1.20645	1.18284	1.42956	1.42846	1.48258	1.41717
1.10E+01	1.44702	1.40578	1.46126	1.41074	1.17348	1.15037	1.39359	1.39246	1.44629	1.38169
1.20E+01	1.41189	1.37192	1.42510	1.37557	1.14266	1.12022	1.35977	1.35857	1.41184	1.34822
1.30E+01	1.37914	1.34039	1.39152	1.34296	1.11424	1.09220	1.32827	1.32704	1.37964	1.31704
1.40E+01	1.34915	1.31148	1.36088	1.31321	1.08819	1.06671	1.29949	1.29819	1.35010	1.28849
1.50E+01	1.32194	1.28519	1.33312	1.28625	1.06475	1.04373	1.27338	1.27206	1.32326	1.26262
1.60E+01	1.29684	1.26093	1.30755	1.26152	1.04329	1.02251	1.24929	1.24798	1.29848	1.23877
1.80E+01	1.25301	1.21851	1.26283	1.21821	1.00584	0.98577	1.20709	1.20578	1.25514	1.19699
2.00E+01	1.21456	1.18122	1.22373	1.18035	0.97344	0.95414	1.17014	1.16882	1.21704	1.16038
2.20E+01	1.18093	1.14863	1.18954	1.14725	0.94534	0.92650	1.13777	1.13647	1.18368	1.12832
2.40E+01	1.15191	1.12041	1.15998	1.11865	0.92092	0.90250	1.10976	1.10841	1.15486	1.10056
2.60E+01	1.12558	1.09488	1.13327	1.09282	0.89917	0.88107	1.08443	1.08311	1.12869	1.07547
2.80E+01	1.10235	1.07232	1.10971	1.07006	0.87987	0.86220	1.06206	1.06075	1.10558	1.05331
3.00E+01	1.08101	1.05164	1.08816	1.04926	0.86238	0.84507	1.04158	1.04030	1.08433	1.03301
4.00E+01	1.00157	0.97448	1.00783	0.97160	0.79706	0.78113	0.96517	0.96391	1.00516	0.95726
5.00E+01	0.94790	0.92232	0.95365	0.91931	0.75344	0.73831	0.91354	0.91242	0.95157	0.90615
6.00E+01	0.90919	0.88469	0.91469	0.88174	0.72214	0.70762	0.87637	0.87514	0.91288	0.86916
8.00E+01	0.85682	0.83373	0.86177	0.83071	0.67995	0.66627	0.82584	0.82480	0.86049	0.81920
1.00E+02	0.82277	0.80058	0.82744	0.79764	0.65265	0.63950	0.79303	0.79191	0.82640	0.78659
1.50E+02	0.77352	0.75263	0.77771	0.74970	0.61332	0.60093	0.74547	0.74445	0.77706	0.73950
2.00E+02	0.74653	0.72635	0.75052	0.72338	0.59184	0.57986	0.71944	0.71845	0.75000	0.71370
3.00E+02	0.71714	0.69777	0.72092	0.69485	0.56852	0.55703	0.69109	0.69007	0.72052	0.68555
4.00E+02	0.70127	0.68232	0.70495	0.67936	0.55591	0.54466	0.67578	0.67482	0.70459	0.67040
5.00E+02	0.69117	0.67249	0.69474	0.66950	0.54793	0.53685	0.66600	0.66504	0.69445	0.66071
6.00E+02	0.68406	0.66559	0.68760	0.66260	0.54232	0.53135	0.65915	0.65817	0.68732	0.65389
8.00E+02	0.67479	0.65657	0.67824	0.65363	0.53498	0.52417	0.65018	0.64919	0.67801	0.64500
1.00E+03	0.66901	0.65093	0.67238	0.64794	0.53041	0.51967	0.64456	0.64362	0.67219	0.63946
1.50E+03	0.66068	0.64283	0.66401	0.63992	0.52384	0.51324	0.63653	0.63559	0.66382	0.63149
2.00E+03	0.65626	0.63855	0.65954	0.63562	0.52034	0.50983	0.63224	0.63134	0.65939	0.62727
3.00E+03	0.65152	0.63392	0.65479	0.63100	0.51659	0.50614	0.62769	0.62675	0.65462	0.62272
4.00E+03	0.64895	0.63143	0.65220	0.62849	0.51458	0.50419	0.62520	0.62428	0.65205	0.62027
5.00E+03	0.64739	0.62991	0.65064	0.62694	0.51335	0.50294	0.62370	0.62280	0.65047	0.61879
6.00E+03	0.64622	0.62878	0.64947	0.62584	0.51245	0.50207	0.62258	0.62161	0.64929	0.61763
8.00E+03	0.64485	0.62744	0.64807	0.62452	0.51136	0.50097	0.62123	0.62028	0.64792	0.61631
1.00E+04	0.64388	0.62651	0.64706	0.62357	0.51060	0.50023	0.62026	0.61939	0.64694	0.61541
1.50E+04	0.64271	0.62536	0.64590	0.62241	0.50967	0.49932	0.61915	0.61822	0.64577	0.61426
2.00E+04	0.64194	0.62462	0.64512	0.62168	0.50905	0.49877	0.61841	0.61748	0.64499	0.61353
3.00E+04	0.64136	0.62404	0.64451	0.62110	0.50859	0.49827	0.61782	0.61689	0.64441	0.61295
4.00E+04	0.64097	0.62367	0.64412	0.62073	0.50830	0.49800	0.61744	0.61652	0.64401	0.61258
5.00E+04	0.64058	0.62331	0.64381	0.62037	0.50802	0.49772	0.61715	0.61623	0.64362	0.61227
6.00E+04	0.64058	0.62329	0.64373	0.62037	0.50797	0.49768	0.61707	0.61616	0.64362	0.61221
8.00E+04	0.64039	0.62310	0.64358	0.62015	0.50783	0.49754	0.61693	0.61601	0.64343	0.61206
1.00E+05	0.64020	0.62292	0.64335	0.62000	0.50769	0.49741	0.61670	0.61579	0.64324	0.61185

Table S4. Mean free path (MFP, cm) of the hafnium-containing MAX phase borides in the energy range from 1 keV to 100 GeV.

Energy (MeV)	Hf ₂ SB	Hf ₂ SeB	Hf ₂ InB	Hf ₂ TeB	Hf ₂ PbB	Hf ₂ BiB	Hf ₂ InB ₂	Hf ₂ SnB ₂	Hf ₂ PB ₄	Hf ₂ SnB ₄
1.00E-03	0.00003	0.00003	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00003	0.00002
1.50E-03	0.00007	0.00004	0.00005	0.00005	0.00005	0.00004	0.00005	0.00005	0.00007	0.00005
2.00E-03	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003
3.00E-03	0.00006	0.00006	0.00007	0.00006	0.00005	0.00004	0.00006	0.00006	0.00006	0.00006
4.00E-03	0.00011	0.00011	0.00010	0.00013	0.00008	0.00008	0.00010	0.00010	0.00012	0.00011
5.00E-03	0.00020	0.00020	0.00017	0.00015	0.00014	0.00014	0.00016	0.00016	0.00020	0.00017
6.00E-03	0.00031	0.00031	0.00027	0.00024	0.00022	0.00022	0.00026	0.00025	0.00032	0.00026
8.00E-03	0.00064	0.00065	0.00055	0.00050	0.00046	0.00044	0.00053	0.00052	0.00066	0.00055
1.00E-02	0.00045	0.00047	0.00047	0.00045	0.00043	0.00042	0.00046	0.00045	0.00046	0.00045
1.50E-02	0.00082	0.00074	0.00090	0.00087	0.00068	0.00067	0.00087	0.00087	0.00082	0.00083
2.00E-02	0.00173	0.00158	0.00192	0.00184	0.00119	0.00116	0.00185	0.00184	0.00173	0.00177
3.00E-02	0.00502	0.00461	0.00384	0.00536	0.00344	0.00332	0.00370	0.00361	0.00503	0.00386
4.00E-02	0.01071	0.00990	0.00817	0.00742	0.00730	0.00704	0.00785	0.00769	0.01073	0.00821
5.00E-02	0.01920	0.01784	0.01472	0.01333	0.01306	0.01260	0.01415	0.01385	0.01922	0.01477
6.00E-02	0.03070	0.02867	0.02375	0.02149	0.02092	0.02018	0.02281	0.02232	0.03073	0.02377
8.00E-02	0.01440	0.01488	0.01562	0.01499	0.01513	0.01483	0.01501	0.01497	0.01439	0.01446
1.00E-01	0.02545	0.02632	0.02770	0.02659	0.01797	0.01742	0.02661	0.02655	0.02542	0.02562
1.50E-01	0.07111	0.07338	0.07755	0.07452	0.05002	0.04849	0.07440	0.07425	0.07096	0.07162
2.00E-01	0.14190	0.14573	0.15433	0.14848	0.10067	0.09755	0.14779	0.14755	0.14145	0.14252
3.00E-01	0.33393	0.33872	0.35934	0.34649	0.24437	0.23709	0.34271	0.34236	0.33210	0.33219
4.00E-01	0.54572	0.54714	0.58066	0.56083	0.41315	0.40157	0.55175	0.55147	0.54159	0.53755
5.00E-01	0.74444	0.73963	0.78478	0.75898	0.58013	0.56486	0.74364	0.74358	0.73762	0.72745
6.00E-01	0.92132	0.90930	0.96461	0.93361	0.73454	0.71621	0.91223	0.91239	0.91180	0.89497
8.00E-01	1.21936	1.19322	1.26520	1.22581	1.00232	0.97944	1.19350	1.19409	1.20494	1.17534
1.00E+00	1.46530	1.42687	1.51254	1.46632	1.22723	1.20085	1.42478	1.42568	1.44667	1.40605
1.50E+00	1.91298	1.85381	1.96336	1.90435	1.63262	1.60010	1.84734	1.84875	1.88742	1.82711
2.00E+00	2.16178	2.09396	2.21465	2.14751	1.84490	1.80862	2.08526	2.08667	2.13449	2.06336
3.00E+00	2.38110	2.30798	2.43214	2.35618	2.01257	1.97342	2.29589	2.29667	2.35656	2.27260
4.00E+00	2.43189	2.35903	2.47774	2.39828	2.03623	1.99673	2.34460	2.34471	2.41230	2.32148
5.00E+00	2.41560	2.34437	2.45576	2.37532	2.00672	1.96773	2.32836	2.32796	2.40062	2.30610
6.00E+00	2.37161	2.30252	2.40710	2.32704	1.95769	1.91959	2.28577	2.28499	2.36049	2.26444
7.00E+00	2.31605	2.24890	2.34738	2.26840	1.90227	1.86493	2.23181	2.23068	2.30796	2.21143
8.00E+00	2.25685	2.19179	2.28473	2.20710	1.84604	1.80988	2.17442	2.17307	2.25116	2.15495
9.00E+00	2.19787	2.13472	2.22283	2.14680	1.79181	1.75656	2.11724	2.11582	2.19409	2.09868
1.00E+01	2.14117	2.07992	2.16380	2.08928	1.74054	1.70648	2.06242	2.06083	2.13892	2.04454
1.10E+01	2.08761	2.02811	2.10816	2.03527	1.69298	1.65963	2.01053	2.00889	2.08656	1.99336
1.20E+01	2.03692	1.97927	2.05599	1.98453	1.64851	1.61614	1.96173	1.96000	2.03686	1.94506
1.30E+01	1.98968	1.93378	2.00753	1.93748	1.60752	1.57571	1.91629	1.91451	1.99040	1.90008
1.40E+01	1.94642	1.89206	1.96333	1.89456	1.56993	1.53894	1.87477	1.87289	1.94779	1.85890
1.50E+01	1.90715	1.85414	1.92328	1.85567	1.53612	1.50579	1.83710	1.83519	1.90906	1.82157
1.60E+01	1.87095	1.81914	1.88640	1.81999	1.50516	1.47516	1.80235	1.80046	1.87331	1.78716
1.80E+01	1.80771	1.75794	1.82187	1.75751	1.45112	1.42217	1.74147	1.73957	1.81079	1.72690
2.00E+01	1.75224	1.70414	1.76547	1.70288	1.40437	1.37654	1.68815	1.68626	1.75582	1.67408
2.20E+01	1.70373	1.65713	1.71614	1.65514	1.36384	1.33666	1.64146	1.63957	1.70770	1.62783
2.40E+01	1.66185	1.61642	1.67349	1.61387	1.32861	1.30204	1.60104	1.59910	1.66612	1.58778
2.60E+01	1.62386	1.57958	1.63496	1.57661	1.29723	1.27112	1.56450	1.56259	1.62835	1.55158
2.80E+01	1.59035	1.54703	1.60097	1.54377	1.26939	1.24389	1.53223	1.53034	1.59501	1.51961
3.00E+01	1.55956	1.51719	1.56988	1.51376	1.24415	1.21918	1.50269	1.50083	1.56436	1.49032
4.00E+01	1.44495	1.40588	1.45399	1.40173	1.14992	1.12693	1.39245	1.39064	1.45014	1.38104
5.00E+01	1.36754	1.33063	1.37582	1.32629	1.08699	1.06516	1.31796	1.31635	1.37283	1.30729
6.00E+01	1.31169	1.27634	1.31961	1.27209	1.04183	1.02088	1.26433	1.26256	1.31701	1.25394
8.00E+01	1.23613	1.20282	1.24327	1.19846	0.98096	0.96122	1.19143	1.18994	1.24142	1.18185
1.00E+02	1.18701	1.15499	1.19374	1.15076	0.94157	0.92261	1.14410	1.14249	1.19224	1.13481
1.50E+02	1.11595	1.08581	1.12200	1.08159	0.88483	0.86696	1.07549	1.07402	1.12106	1.06688
2.00E+02	1.07701	1.04790	1.08277	1.04362	0.85384	0.83657	1.03794	1.03651	1.08202	1.02965
3.00E+02	1.03461	1.00666	1.04007	1.00245	0.82020	0.80362	0.99703	0.99556	1.03949	0.98904
4.00E+02	1.01172	0.98438	1.01702	0.98011	0.80201	0.78578	0.97495	0.97356	1.01651	0.96718
5.00E+02	0.99715	0.97019	1.00230	0.96588	0.79050	0.77452	0.96084	0.95945	1.00189	0.95320
6.00E+02	0.98689	0.96024	0.99199	0.95593	0.78240	0.76657	0.95096	0.94953	0.99159	0.94337
8.00E+02	0.97352	0.94723	0.97849	0.94299	0.77182	0.75621	0.93801	0.93659	0.97816	0.93053
1.00E+03	0.96518	0.93910	0.97003	0.93479	0.76522	0.74973	0.92990	0.92855	0.96977	0.92255
1.50E+03	0.95315	0.92741	0.95797	0.92320	0.75574	0.74044	0.91833	0.91697	0.95769	0.91105
2.00E+03	0.94679	0.92123	0.95151	0.91701	0.75069	0.73553	0.91213	0.91083	0.95131	0.90496
3.00E+03	0.93994	0.91456	0.94467	0.91035	0.74528	0.73021	0.90556	0.90421	0.94441	0.89840
4.00E+03	0.93624	0.91097	0.94093	0.90671	0.74238	0.72739	0.90197	0.90065	0.94070	0.89486
5.00E+03	0.93398	0.90876	0.93867	0.90448	0.74060	0.72560	0.89981	0.89851	0.93842	0.89272
6.00E+03	0.93230	0.90713	0.93698	0.90290	0.73930	0.72433	0.89819	0.89680	0.93673	0.89105
8.00E+03	0.93032	0.90521	0.93497	0.90100	0.73774	0.72274	0.89625	0.89488	0.93475	0.88914
1.00E+04	0.92892	0.90386	0.93351	0.89962	0.73665	0.72169	0.89485	0.89360	0.93334	0.88785
1.50E+04	0.92724	0.90221	0.93184	0.89794	0.73529	0.72037	0.89325	0.89190	0.93165	0.88619
2.00E+04	0.92613	0.90114	0.93072	0.89689	0.73441	0.71958	0.89217	0.89084	0.93052	0.88513
3.00E+04	0.92529	0.90030	0.92983	0.89605	0.73373	0.71886	0.89132	0.88999	0.92968	0.88430
4.00E+04	0.92472	0.89976	0.92927	0.89553	0.73333	0.71846	0.89078	0.88946	0.92911	0.88377
5.00E+04	0.92416	0.89924	0.92882	0.89500	0.73292	0.71806	0.89035	0.88903	0.92855	0.88332
6.00E+04	0.92416	0.89922	0.92871	0.89500	0.73285	0.71800	0.89025	0.88893	0.92855	0.88324
8.00E+04	0.92388	0.89895	0.92849	0.89469	0.73265	0.71780	0.89004	0.88872	0.92827	0.88301
1.00E+05	0.92361	0.89868	0.92816	0.89448	0.73245	0.71761	0.88971	0.88840	0.92799	0.88271

Because high Z A-site elements simultaneously increase both Z_{eff} and density, their attenuation advantages become amplified once the density is taken into account.

to HfB_2 (39.05 cm^{-1}). The density contribution therefore enhances the compositional contrast observed in the MAC, where the difference was approximately 25%.

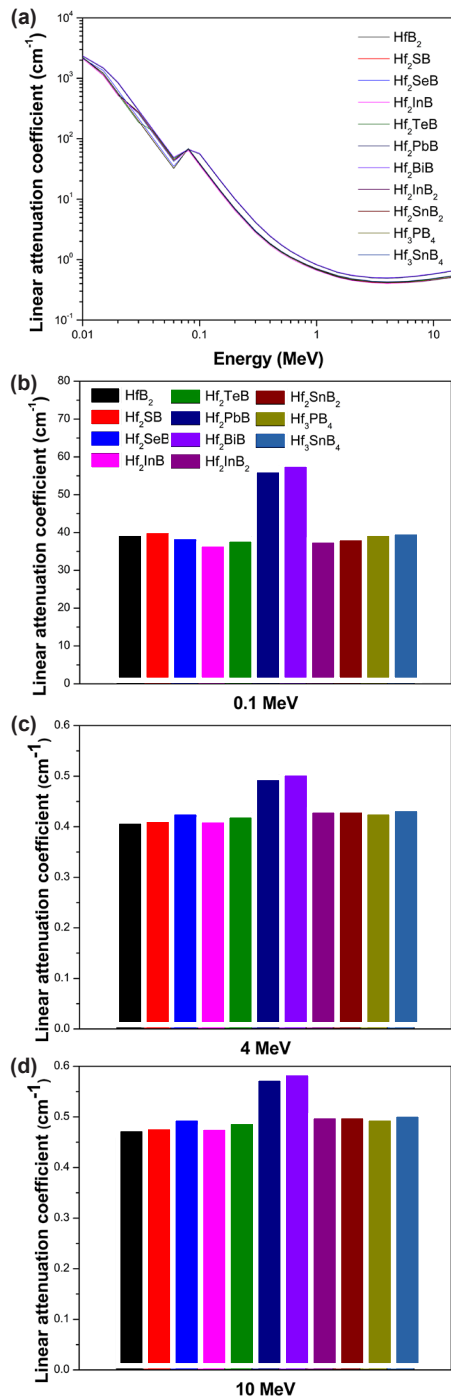


Figure 2. (a) LAC as a function of incident photon energy for Hf_2SB , Hf_2SeB , Hf_2InB , Hf_2TeB , Hf_2PbB , Hf_2BiB , Hf_2InB_2 , Hf_2SnB_2 , Hf_3PB_4 , Hf_3SnB_4 , and HfB_2 . LAC values at specific energies: (b) 0.1 MeV, (c) 4 MeV, and (d) 10 MeV.

As seen in Figure 2a, this effect becomes particularly evident at low photon energies. Indeed, at 0.1 MeV, where photoelectric absorption dominates, Hf_2BiB exhibits the highest LAC value (57.40 cm^{-1}), followed closely by Hf_2PbB at 55.65 cm^{-1} . These values correspond to increases of 47.0% and 42.5% compared

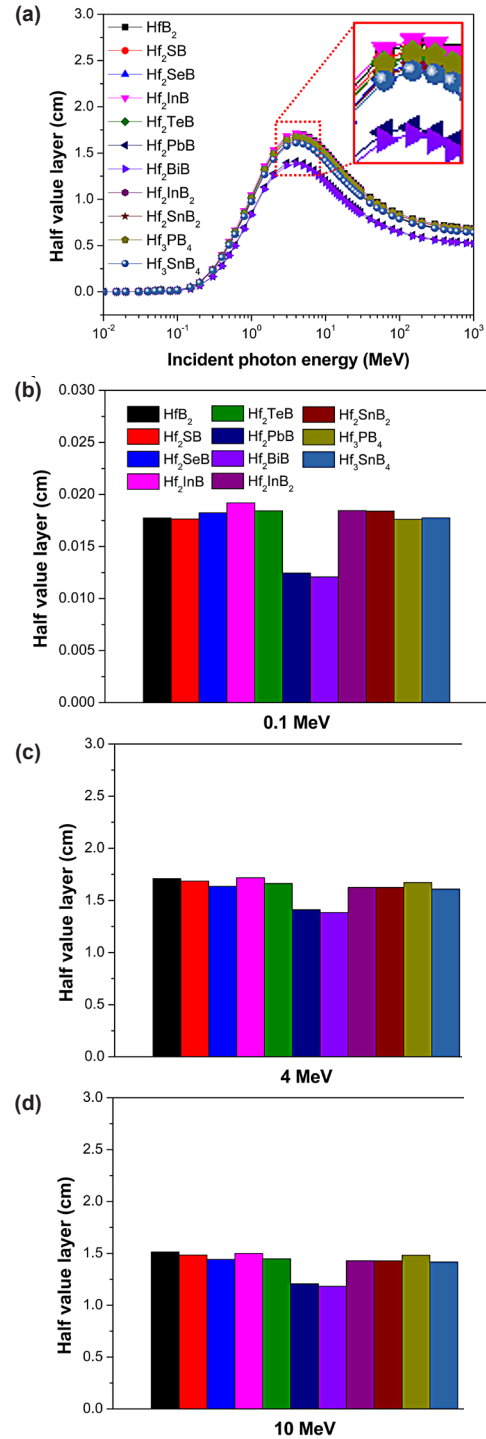


Figure 3. (a) HVL as a function of incident photon energy for Hf_2SB , Hf_2SeB , Hf_2InB , Hf_2TeB , Hf_2PbB , Hf_2BiB , Hf_2InB_2 , Hf_2SnB_2 , Hf_3PB_4 , Hf_3SnB_4 , and HfB_2 . HVL values at specific energies: (b) 0.1 MeV, (c) 4 MeV, and (d) 10 MeV.

The higher LACs of Bi- and Pb-containing phases translate into significantly thinner required shielding, with HVLs of 0.01208 cm and 0.01245 cm, representing reductions of 31.9% and 29.9% relative to HfB_2 (0.01775 cm) (Figure 3b). Their MFPs, measured as

0.01742 cm and 0.01797 cm, show similar proportional improvements as seen in (Figure 4b).

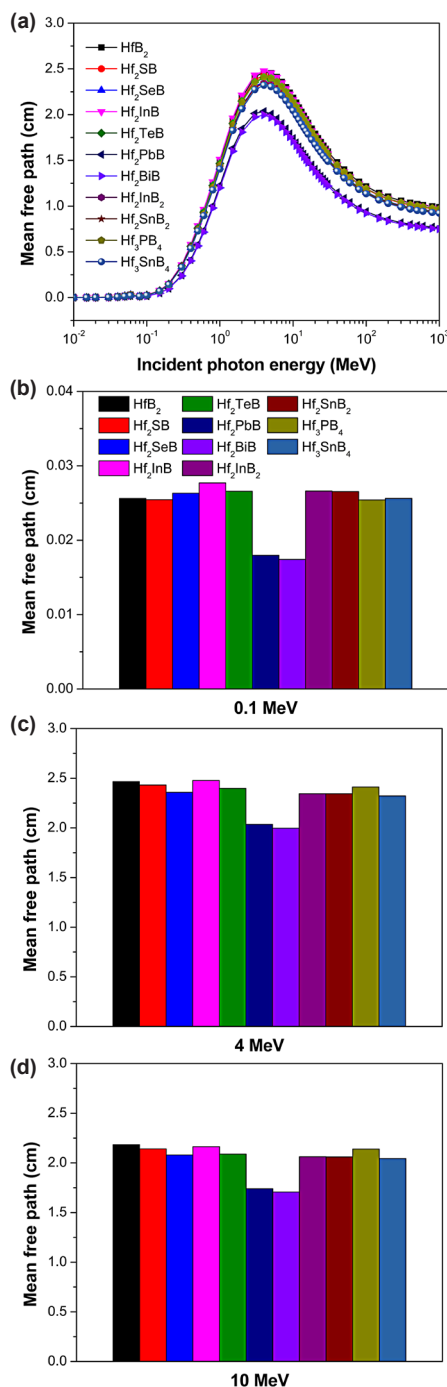


Figure 4. (a) MFP as a function of incident photon energy for Hf₂SB, Hf₂SeB, Hf₂InB, Hf₂TeB, Hf₂PbB, Hf₂BiB, Hf₂InB₂, Hf₂SnB₂, Hf₃PB₄, Hf₃SnB₄, and HfB₂. MFP values at specific energies: (b) 0.1 MeV, (c) 4 MeV, and (d) 10 MeV.

MAX phases with lighter A-site elements, particularly Hf₂SB and Hf₃PB₄, also show strong low-energy performance despite their relatively lower densities compared to other MAX-phases (Table 1). At 0.1 MeV, Hf₂SB exhibits LAC=39.29 cm⁻¹, HVL=0.01764 cm, and MFP=0.02545 cm, while Hf₃PB₄ records LAC=39.34 cm⁻¹, HVL=0.01762 cm,

and MFP=0.02542 cm. These values are slightly better than those of HfB₂ and indicate that preserving high Hf content in selected light-A-site compositions can maintain effective photon attenuation even without heavy A-site elements.

In the intermediate Compton-scattering region (~3-6 MeV), LAC values converge to 0.40-0.50 cm⁻¹, as seen in Figure 2c. Nonetheless, Bi- and Pb-containing phases maintain a modest residual advantage, with LAC(Bi)=0.501 cm⁻¹ and LAC(Pb)=0.491 cm⁻¹, while HVLs (1.384 cm and 1.411 cm) and MFPs (1.997 cm and 2.036 cm) remain ≈18-19 % shorter than HfB₂ (HVL=1.710 cm, MFP=2.467 cm) (Figures 3c and 4c). Furthermore, most MAX-related borides show higher calculated LAC values than HfB₂ in this regime, with the only exception being Hf₂InB (LAC=0.404 cm⁻¹), which is marginally below HfB₂ due to its slightly lower density.

As seen in Figure 2d, at 10 MeV, where pair production contributes significantly, LAC values increase slightly (0.46-0.59 cm⁻¹), and all MAX-related borides now surpass HfB₂ (0.458 cm⁻¹). Hf₂BiB (0.586 cm⁻¹) and Hf₂PbB (0.575 cm⁻¹) remain the top performers, with HVLs of 1.183 cm and 1.206 cm and MFPs of 1.706 cm and 1.741 cm, corresponding to 20-22 % reductions relative to HfB₂ (HVL=1.513 cm; MFP=2.183 cm) (Figures 3d and 4d). The remaining MAX phases, including Hf₂TeB, Hf₂InB, Hf₂SB, and Hf₃SnB₄, also show improved attenuation, with HVLs between 1.42-1.48 cm and MFPs below HfB₂, reflecting 3-6 % improvements. These results indicate that, at intermediate and high photon energies, several light- and intermediate-Z A-site compositions achieve improved calculated shielding performance compared with the conventional binary boride, highlighting the combined influence of density, elemental composition, and boron/Hf ratio.

Furthermore, the overall γ-ray shielding performance of the Hf-containing MAX-related borides was quantitatively benchmarked against elemental Pb (ρ=11.34 g.cm⁻³), the conventional reference material, in terms of HVL and MFP. As shown in Table 3, Hf₂BiB and Hf₂PbB exhibit calculated HVL and MFP values comparable to Pb and, at selected intermediate and high photon energies, slightly lower than those of Pb. Indeed, at 662 keV, Hf₂BiB (0.556 cm) and Hf₂PbB (0.570 cm) exhibit HVLs nearly identical to Pb (0.555 cm). At intermediate energies (1173 and 1332 keV), Hf₂BiB (0.947 cm and 1.035 cm) and Hf₂PbB (0.967 cm and 1.057 cm) show 2.3% to 5.0% lower calculated HVLs than Pb (0.990 cm and 1.089 cm), indicating a modest calculated shielding advantage under these specific conditions. At 2506 keV, Hf₂BiB (1.331 cm) and Hf₂PbB (1.356 cm) also show lower calculated HVL values than Pb (1.404 cm), indicating improved calculated γ-ray attenuation at this specific energy.

Table 3. HVL and MFP values for Hf-containing MAX-related borides in comparison with HfB₂ and Pb at specific energies of 662 keV, 1173 keV, 1332 keV, and 2506 keV.

Sample	Half value layer (cm)				Mean free path (cm)			
	662 keV	1173 keV	1332 keV	2506 keV	662 keV	1173 keV	1332 keV	2506 keV
Hf ₂ SB	0.707	1.143	1.242	1.597	1.020	1.649	1.791	2.305
Hf ₂ SeB	0.696	1.110	1.204	1.548	1.004	1.602	1.737	2.233
Hf ₂ InB	0.738	1.176	1.276	1.634	1.065	1.697	1.840	2.357
Hf ₂ PbB	0.570	0.967	1.057	1.356	0.823	1.396	1.524	1.957
Hf ₂ BiB	0.556	0.947	1.035	1.331	0.803	1.367	1.494	1.920
Hf ₂ TeB ₂	0.715	1.141	1.237	1.584	1.031	1.646	1.785	2.285
Hf ₂ InB	0.697	1.107	1.200	1.540	1.006	1.598	1.732	2.222
Hf ₂ SnB ₂	0.698	1.108	1.201	1.541	1.006	1.599	1.733	2.224
Hf ₂ PB ₂	0.700	1.128	1.225	1.579	1.009	1.628	1.767	2.278
Hf ₃ SnB ₄	0.685	1.094	1.187	1.525	0.988	1.579	1.712	2.200
HfB ₂	0.714	1.155	1.254	1.617	1.030	1.666	1.809	2.332
Pb	0.5547	0.9898	1.0890	1.4044	0.800	1.428	1.571	2.026

It should be emphasized that the calculated advantage over Pb is not universal across all photon energies and shielding descriptors. Rather, it is observed for selected compositions, particularly Hf₂BiB and Hf₂PbB, at specific intermediate and high-energy γ -ray conditions in terms of HVL and MFP. Besides, although Hf₂PbB contains a lower Pb fraction than elemental Pb, it is not a completely Pb-free composition because Pb is still present as an A-site element. Therefore, Hf₂PbB is discussed mainly to illustrate the effect of partial heavy A-site incorporation on γ -ray attenuation, whereas Hf₂BiB represents the more relevant Pb-free high-Z candidate among the investigated compositions.

Pb is commonly used as a benchmark γ -ray shielding material because of its high atomic number and density. While Hf₂PbB contains the heavy Pb atom, it also incorporates lower-Z elements, namely Hf (Z=72) and B (Z=5). This compositional dilution would normally be expected to reduce the effective atomic number and attenuation efficiency relative to elemental Pb. However, the hexagonal layered MAX-related crystal structures can contribute to efficient atomic packing and high bulk density, thereby increasing the number of interacting atoms and electrons per unit volume. Therefore, the improved γ -ray attenuation should be interpreted as the combined effect of crystal-structure-related density, elemental composition, Hf content, and heavy A-site chemistry rather than as an intrinsic consequence of the MAX structure alone. As a result, selected dense compositions, particularly Hf₂BiB and Hf₂PbB, show calculated LAC, HVL, and MFP values comparable to or slightly better than Pb at specific photon energies.

Of further note, the performance gap between the remaining MAX phases and Pb narrows substantially with increasing photon energy. For example, Hf₂SB,

which requires a 0.707 cm layer at 662 keV ($\approx 27.5\%$ thicker than Pb), reduces this difference to $\approx 13.7\%$ at 2506 keV (1.597 cm vs. 1.404 cm). Similarly, Hf₂SnB₄ decreases from a 23.5% HVL excess at 662 keV (0.685 cm vs. 0.555 cm) to less than 9% at 2506 keV (1.525 cm vs. 1.404 cm). The corresponding MFP values follow the same trend (Figure 4), suggesting that several Hf-containing MAX-related borides become increasingly competitive with Pb at higher γ -ray energies due to their relatively high densities.

This convergence is driven by the energy-dependent influence of photon interaction mechanisms. At lower energies, photoelectric absorption contributes more strongly and scales steeply with atomic number, approximately as Z^4 - Z^5 ; therefore, Bi- and Pb-containing phases exhibit lower HVL values than lighter A-site compositions. At intermediate and high energies (≥ 1173 keV), Compton scattering and pair production become more dominant and scale more weakly with atomic number, approximately as Z or Z^2 [49]. In this regime, electron density and density-related packing effects increasingly influence shielding efficiency.

Consequently, lighter A-site compositions such as Hf₂SB, Hf₃PB₄, Hf₂SeB, and Hf₃SnB₄ become more competitive at higher photon energies despite their lower atomic numbers. This trend may be advantageous for Pb-reduced shielding concepts, although practical benefits related to toxicity, mechanical behavior, and thermal stability require experimental validation.

Overall, these findings indicate that several Hf-containing MAX-related borides can outperform conventional HfB₂ within selected photon-energy ranges and attenuation parameters. High-Z A-site substitutions, such as Bi and Pb, provide the strongest calculated γ -ray attenuation among the investigated compositions, benefiting from both elevated atomic number and density, while light-A-site compositions such as Hf₂SB and Hf₃PB₄ retain effective low-energy performance through preserved Hf content. Intermediate-Z and B-rich MAX-related borides show improved performance relative to HfB₂ at medium and high energies, achieving lower HVLs and MFPs under these conditions. This collective behavior highlights the dual role of A-site chemistry and bulk density in governing γ -ray shielding, indicating that MAX-related borides provide a tunable compositional platform for compact and multifunctional radiation-shielding applications. Although the present γ -ray shielding evaluation focuses on MAC, LAC, HVL, MFP, and Z_{eff} , additional application-oriented parameters such as exposure buildup factor (EBF), energy absorption buildup factor (EABF), radiation protection efficiency (RPE), and transmission factor may provide further insight into thickness- and geometry-dependent shielding performance. These parameters should therefore be considered in future detailed shielding-design studies.

Beyond γ -shielding, the charged particle attenuation capabilities of Hf-containing MAX-related borides were also evaluated. Unlike uncharged photons, energetic charged particles interact with matter primarily through Coulombic forces. As they traverse the material, the Coulomb fields of these incident particles perturb the electron clouds and atomic nuclei of the absorbing medium, leading to continuous energy deposition. The efficiency of this energy transfer, and thus the penetration depth, is profoundly dependent on the projectile's properties such as its charge, mass, and kinetic energy [49,52].

Figure 5 illustrates the range of protons, alpha particles, and electrons in the studied materials across a kinetic energy range of 0.1-10 MeV. The range of a charged particle represents the penetration depth it can achieve before losing its energy through ionization and excitation processes. A lower calculated range indicates stronger stopping capability for the corresponding charged particle, which is desirable for radiation-shielding applications. It is evident

that the particle range consistently increases with kinetic energy for all types of charged particles, as higher-energy particles require a greater path length to dissipate their energy within the material.

A clear observation from Figure 5 is the distinct hierarchy in penetration depths: electrons exhibit significantly greater ranges than protons, which in turn penetrate much deeper than alpha particles at identical kinetic energies. For instance, at 5 MeV, the range for electrons in these borides is typically between approximately 2960 and 3475 μm , while protons are stopped within a much shorter distance of about 83 to 93 μm , and alpha particles show the shortest ranges, approximately 10.9 to 12.5 μm . This difference is intrinsically linked to the particle's mass and charge. Protons and alpha particles, being considerably heavier, primarily lose energy through inelastic Coulombic interactions with the atomic electrons of the medium. Their large mass limits deflections, leading to relatively straight trajectories and effective energy transfer. Alpha particles, with a $+2e$ charge, experience

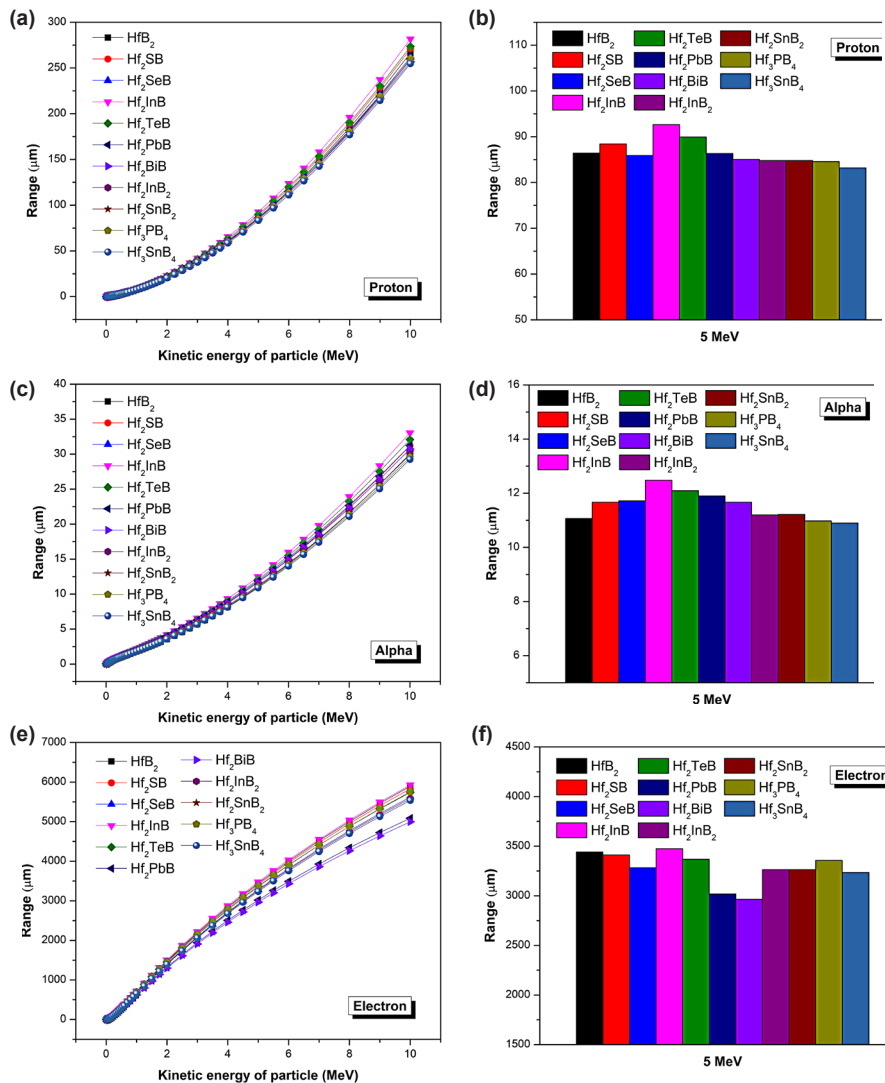


Figure 5. Comparative analysis of charged particle ranges in Hf-containing MAX-related borides, in comparison with the conventional binary boride HfB₂. (a) and (b) display the proton range as a function of kinetic energy and at 5 MeV, respectively. (c) and (d) illustrate the alpha particle range as a function of kinetic energy and at 5 MeV, respectively. (e) and (f) present the electron range as a function of kinetic energy and at 5 MeV, respectively. A lower calculated range indicates stronger stopping capability.

a fourfold increase in stopping power compared to protons (+1e) at the same velocity, leading to their comparatively shorter ranges. Electrons, conversely, are light and undergo both collisional (ionization/excitation) and radiative (bremsstrahlung) energy losses. The latter, resulting from deceleration in the strong nuclear fields, becomes increasingly dominant at higher energies and in high-Z materials like those containing both Hf and Bi or Pb. Therefore, the specific composition of each Hf-containing MAX-related boride critically influences its ability to attenuate charged particles, as reflected in their varying ranges at a given energy.

For 5 MeV electrons, the decreasing projected range order is: Hf_2InB (3475.10 μm) > HfB_2 (3441 μm) > Hf_2SB (3411.77 μm) > Hf_2TeB (3367.99 μm) > Hf_3PB_4 (3357.88 μm) > Hf_2InB_2 (3263.06 μm) $\approx$ Hf_2SnB_2 (3263.49 μm) > Hf_2SeB (3283.65 μm) > Hf_3SnB_4 (3235.50 μm) > Hf_2PbB (3018.11 μm) > Hf_2BiB (2965.96 μm) (Figure 5f). The shorter calculated electron range in Hf_2BiB is primarily attributable to the presence of very high-Z Bi in its composition. This high atomic number can enhance the radiative stopping-power component through bremsstrahlung processes, which strongly depend on Z^2 , thereby contributing to shorter calculated electron ranges [49,52].

Conversely, protons and alpha particles interact primarily through electronic stopping, leading to a notable re-ordering of performance. For protons at 5 MeV (Figure 5b), the boron-rich phases, Hf_3SnB_4 (83.18 μm) and Hf_3PB_4 (84.6 μm), provide the shortest calculated ranges among the investigated compositions. The trend is consistent for alpha particles (Figure 5d), where Hf_3SnB_4 (10.9 μm) again records the shortest range. This observation indicates that, for heavy charged particles, the high-Z and density advantage of Hf_2PbB and Hf_2BiB is less dominant than it is for γ -ray attenuation. Electronic stopping is instead more sensitive to the material's mean excitation energy (I-value) and ratio. The higher I-values associated with elements like Bi and Pb imply more tightly bound atomic electrons, which reduce the efficiency of energy transfer via ionization. Consequently, the boron-rich Hf_3SnB_4 and Hf_3PB_4 phases provide shorter calculated ranges for protons and alpha particles, suggesting more favorable stopping behavior for heavy charged particles within the investigated composition space.

Neutron shielding performance of the Hf-containing MAX-related borides was evaluated across both fast and thermal energy regimes. Fast neutron attenuation is governed primarily by non-elastic scattering events that remove neutrons from the uncollided flux. The efficiency of this process, measured by the FNRCS, shows a strong compositional dependence across the MAX phases, with performance strongly determined by the material's boron content, as seen in Figure 6.

Consequently, Hf_3PB_4 (0.1647 cm^{-1}) and Hf_3SnB_4

(0.1625 cm^{-1}) exhibit the highest removal cross sections, followed by Hf_2InB_2 (0.1538 cm^{-1}).

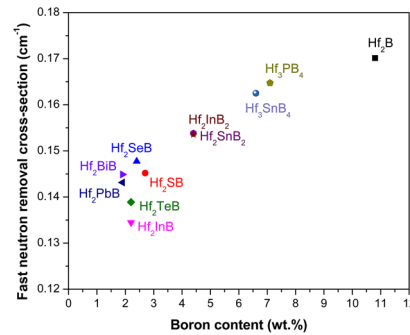


Figure 6. Correlation between boron content and fast neutron removal cross-section of the Hf-containing MAX-related borides, including Hf_2SB , Hf_2SeB , Hf_2InB , Hf_2TeB , Hf_2PbB , Hf_2BiB , Hf_2InB_2 , Hf_2SnB_2 , Hf_3PB_4 , and Hf_3SnB_4 , in comparison with the conventional binary boride HfB_2 .

Although the MAX-related borides exhibit slightly lower FNRCS values than the binary HfB_2 (0.1701 cm^{-1}), this decrease can be ascribed to their comparatively lower boron concentration, which diminishes the overall probability of neutron scattering interactions. Nonetheless, the investigated compounds show strong calculated fast-neutron attenuation and exceed the benchmark FNRCS values used here for B_4C (0.141 cm^{-1}), concrete (0.094 cm^{-1}), and graphite (0.077 cm^{-1}).

In stark contrast to γ -ray shielding, bulk density and high-Z are secondary factors in the fast neutron regime; the overall stopping capability hinges instead on the concentration of light nuclei like boron. This compositional dependence is also observed in thermal neutron absorption, which is strongly influenced by the intrinsic neutron-capture ability of the ^{10}B isotope through the $^{10}\text{B}(n, \alpha)^7\text{Li}$ reaction. Since natural boron contains approximately 19.9% ^{10}B , the present calculations represent natural-isotopic-abundance conditions. Enrichment in ^{10}B would be expected to substantially increase thermal neutron absorption, particularly for the boron-rich Hf_3AB_4 and Hf_2AB_2 compositions. The calculated Σ_a values (total LAC) reveal a distinct compositional dependence, where boron-rich phases exhibit enhanced absorption compared with those containing heavier A-site elements. The thermal absorption ranking follows the structural families: Hf_3AB_4 phases (Hf_3PB_4 : 35.86 cm^{-1} , Hf_3SnB_4 : 32.76 cm^{-1}) Hf_2AB_2 phases (Hf_2InB_2 : 26.25 cm^{-1} , Hf_2SnB_2 : 23.49 cm^{-1}) > Hf_2AB phases (Hf_2SB : 15.44 cm^{-1} , Hf_2InB : 15.24 cm^{-1} , Hf_2SeB : 14.73 cm^{-1} , Hf_2TeB : 12.95 cm^{-1}). This anti-correlation culminates with the heavy-element-containing phases, such as Hf_2BiB (12.58 cm^{-1}) and Hf_2PbB (12.42 cm^{-1}), which register the lowest absorption values. This trend arises because the incorporation of heavy A-site elements such as Bi and Pb reduces the relative concentration of boron-containing neutron-capture centers and therefore lowers the calculated thermal neutron absorption compared with more boron-rich phases.

It should also be noted that these thermal neutron absorption values were calculated for natural isotopic abundances and monoenergetic thermal neutrons. Therefore, direct comparison with isotope-enriched commercial neutron absorbers, particularly ^{10}B -enriched B_4C , should be made with caution.

Overall, the Hf-containing MAX-related borides exhibit a promising dual-regime neutron-shielding response in which performance is governed more strongly by boron concentration and neutron-capture characteristics than by the density factors that dominate γ -ray attenuation. Boron-rich compositions provide higher calculated fast-neutron removal and thermal-neutron absorption, while the presence of naturally absorbing Hf isotopes may further contribute to thermal neutron attenuation. These results highlight the theoretical potential of Hf-containing MAX-related borides as compact multifunctional neutron-shielding candidates.

Compared with recently reported multifunctional shielding systems such as polymer/high-Z particle composites, boron-containing polymer composites, high-Z oxide glasses, and metallic shielding alloys, Hf-containing MAX-related borides offer a different design strategy based on crystalline compounds that combine high-Z elements and neutron-interacting boron within the same material framework. While polymer composites benefit from lightweight processability and glasses or metallic alloys benefit from broad compositional flexibility, the present boride systems may offer compact attenuation performance together with potentially higher thermal stability. However, unlike many experimentally demonstrated composites and glasses, several compositions evaluated here remain theoretically predicted and therefore require experimental validation.

Indeed, the present study is a theoretical screening based on database-derived photon, neutron, and charged-particle interaction parameters. Therefore, the results should be interpreted as comparative predicted shielding trends rather than experimentally validated performance values. The calculations are based on idealized nominal compositions and reported theoretical or experimental density values, whereas experimentally synthesized MAX and MAX-related borides may contain secondary phases, residual reactants, porosity, or compositional deviations depending on the synthesis and densification conditions. In practical applications, shielding performance alone is not sufficient for material deployment; long-term structural stability, radiation tolerance, oxidation resistance, manufacturability, phase assemblage, porosity, grain size, texture, secondary phases, and densification level may also critically affect the final performance. Future validation should therefore include synthesis of the most promising candidates, quantitative phase analysis by X-ray diffraction (XRD)/Rietveld refinement, microstructural characterization, density/porosity measurements, irradiation stability

assessment, and direct γ -ray and neutron attenuation tests.

4. Conclusions

This study systematically evaluated the calculated γ -ray, charged-particle, and neutron attenuation behaviors of Hf-containing MAX-related borides across the Hf_3AB_4 , Hf_2AB_2 , and Hf_2AB families. The results indicate that A-site chemistry, boron concentration, Hf fraction, and density collectively influence attenuation properties, positioning Hf-containing MAX-related borides as promising candidates for further investigation in multifunctional radiation-shielding applications.

The findings clarify the compositional trade-offs governing the calculated attenuation performance. For γ -rays, attenuation behavior is distinctly energy-dependent rather than purely determined by density or atomic number. Heavy A-site compositions such as Hf_2BiB and Hf_2PbB exhibit the strongest calculated γ -ray attenuation among the investigated compositions and show lower HVL values than pure Pb at selected intermediate and high photon energies due to their high effective atomic number and density. However, at lower photon energies, where the photoelectric effect dominates, selected lighter A-site compositions, particularly Hf_2SB and Hf_3PB_4 , retain competitive attenuation by maintaining a high Hf fraction and a favorable compositional contribution to photon absorption. As photon energy increases into the Compton and pair-production regimes, several MAX-related borides show improved calculated performance relative to HfB_2 , with intermediate-Z compositions gaining a relative advantage. This indicates that attenuation efficiency in these materials arises from a complex interplay between atomic composition, density, and energy regime.

For neutron attenuation, both fast and thermal shielding efficiencies scale primarily with boron concentration, while A-site chemistry introduces an additional fine-tuning effect. Among the investigated MAX-related borides, the boron-rich Hf_3AB_4 family, particularly Hf_3PB_4 , achieved the highest fast neutron removal cross section (0.1647 cm^{-1}), exceeding the B_4C benchmark value used in this study. Within this family, compositions with lighter A-site elements further enhanced neutron attenuation efficiency, reflecting the combined influence of high boron content and favorable neutron scattering from lower-Z constituents, whereas material density played a relatively minor role. A similar compositional sensitivity was observed for charged-particle shielding: while Hf_2BiB showed the shortest calculated electron range, the Hf_3AB_4 compounds provided shorter calculated ranges for protons and α -particles, where electronic stopping dominates, and the high-Z advantage becomes less significant.

To conclude, this theoretical analysis identifies Hf_3PB_4 as the most balanced multifunctional candidate among the investigated compositions, combining strong calculated neutron and heavy charged-particle attenuation with competitive γ -ray shielding. Hf_3PB_4 is not the best-performing composition in every individual shielding category; for example, Hf_2BiB and Hf_2PbB exhibit stronger γ -ray attenuation, while Hf_2BiB provides the shortest calculated electron range. However, Hf_3PB_4 offers the most balanced multifunctional response by combining high neutron attenuation, favorable proton/alpha stopping behavior, and competitive γ -ray shielding within a single Pb-free composition. Nevertheless, practical deployment of Hf_3PB_4 would require further assessment of synthesis scalability, phase purity, densification behavior, raw-material cost, and long-term stability under irradiation and operating environments. Notably, the prior successful synthesis of related compounds including Hf_2SB , Hf_2SeB , Hf_2TeB , and Hf_2InB_2 supports the broader feasibility of this material family, although direct synthesis and validation of Hf_3PB_4 and Hf_2BiB remain necessary. Future work should therefore focus on the experimental synthesis, phase-purity confirmation, densification, irradiation stability, and direct radiation-shielding validation of Hf_3PB_4 as the most balanced multifunctional candidate and Hf_2BiB as the most promising Pb-free γ -ray shielding candidate predicted in this study.

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6. Author Contribution Statement

Celal Avcıoğlu: Methodology, data analysis and editing, visualization, and writing draft.

7. Conflict of Interest

The author declares that the manuscript was prepared in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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