Supplementary Information

Enthalpies of Formation of Transition Metal Diborides: A First Principles Study

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Figure S1. Atomic volumes of the transition metals considered in the present work.

Figure S2. Enthalpies of formation of anti-ferromagnetic and non-magnetic MnB₂ in the hP3, tP12, hP12, hR6, hP6, and oP6 structures.
Table S1. Values of the formation enthalpies and atomic volumes of the early transition metals diborides.

<table>
<thead>
<tr>
<th></th>
<th>TiB$_2$</th>
<th>VB$_2$</th>
<th>CrB$_2$</th>
<th>MnB$_2$</th>
<th>FeB$_2$</th>
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<tr>
<td></td>
<td>$\Delta h$</td>
<td>V</td>
<td>$\Delta h$</td>
<td>V</td>
<td>$\Delta h$</td>
</tr>
<tr>
<td></td>
<td>kJ/mol of atoms</td>
<td>$\Lambda$</td>
<td>kJ/mol of atoms</td>
<td>$\Lambda$</td>
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<td>hP12-TMB$_2$</td>
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<td>$8.5705$</td>
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<td>$8.5139$</td>
<td>$-70.03$</td>
<td>$7.8477$</td>
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<td>hP12-TMB$_2$</td>
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Table S2. Comparison of the calculated and experimental values of the lattice parameters and internal parameters of some diborides. The experimental values are the more recent one indicated in the Pearson’s Handbook [13]. For the prototypes, the calculated and experimental values are given in Table 1 of the manuscript.

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<th>Compound</th>
<th>Structure</th>
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<th>a (Å)</th>
<th>b (Å)</th>
<th>c (Å)</th>
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