Phase Stability and Physical Properties of Manganese Borides: A First-Principles Study

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Crystal structures of manganese borides in Mn-B systems as follows:

Mn7B3-Mn7C3:

space group: *Pnma;* cell parameters(A°): a = 4.4188, b = 6.9463, c = 12.0201; atom positions: B1: 8d(0.4622, 0.0337, 0.3472), B2: 4c(0.0325, 1/4, 0.5643), Mn1: 8d(0.2534, 0.0611, 0.0198), Mn2: 8d(0.0340, 0.5629, 0.3097), Mn3: 4c(0.2538, 1/4, 0.2052), Mn4: 4c(0.2152, 1/4, 0.4117), Mn5: 4c(0.4613, 1/4, 0.6261).

Mn2B-Re2P:

space group: *Pnma;* cell parameters(A°): a = 4.7381, b = 2.6185, c = 8.8405; atom positions: B: 4c(0.1594, 1/4, 0.1332), Mn1: 4c(0.0543, 1/4, 0.7231), Mn2: 4c(0.2373, 1/4, 0.4569).

Mn2B-Pt2B:

space group: *P*63*/mmc;* cell parameters(A°): a = 2.5916, c = 9.5583; atom positions: B: 2c(1/3, 2/3, 1/4), Mn: 4f(1/3, 2/3, 0.5995).

MnB-NiAs:

space group: *P*63*/mmc ;* cell parameters(A°): a = 2.6389, c = 5.6504; atom positions: B: 2c(1/3, 2/3, 1/4), Mn: 2a(0, 0, 0).

MnB-WC:

space group: *P*-6*m*2*;* cell parameters(A°): a = 2.6399, c = 2.8130; atom positions: B: 1d(1/3, 2/3, 1/2), Mn: 1a(0, 0, 0).

Mn3B2-Mn3N2:

space group: *I*4*/mmc;* cell parameters(A°): a = 2.5725, c = 13.0721; atom positions: B: 4e(0, 0, 0.2150), Mn1: 4e(0, 0, 0.3752), Mn2: 2a(0, 0, 0).

MnB2-RuB2:

space group: *Pmmc;* cell parameters(A°): a = 2.7852, b = 4.3744, c = 3.8392; atom positions: B: 4e(1/4, 0.0484, 0.1337), Mn: 2a(1/4, 1/4, 0.6333).

MnB2-WB2:

space group: *P*63*/mmc;* cell parameters(A°): a = 2.9379, c = 12.3004; atom positions: B1: 4f(1/3, 2/3, 0.0263), B2: 2c(1/3, 2/3, 1/4), B3: 2b(0, 0, 1/4), Mn: 4f(1/3, 2/3, 0.6405).

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