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B2 decomposition of X5Al (X=Sc, Ti, V, Cr, Y, Zr, Nb, and Mo) system, A First-Principles Study PAYAM NOROUZZADEH, MAHDI SANATI, Physics Department, Texas Tech University, Lubbock, TX 79409-1051 — The phase stability of B2 X5Al (X=Sc, Ti, V, Cr, Y, Zr, Nb, and Mo), and slightly rearranged atomic structures are examined by first-principles calculations. The ground state energy calculations show instability against the omega structure type atomic displacement in all of these systems. We use electronic density of states and a rigid band modeling to understand and explain the electronic origin of the stability of each system. In order to estimate the strength of each bond, the heats of formation for several compounds are calculated. We find that the strength of the transition metal (TM)-Al bond increases from Sc to Cr, and Y to Mo. The crystal structure parameters, such as lattice constants and bulk modulus, are calculated.

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