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Electronic and Magnetic Properties of B_5CX (X=V, Cr, Mn, Fe, Ni, and Co): a Theoretical Study DAYNE SHIELDS, Department of Physics, University of Nebraska at Omaha, WAI-NING MEI, JING LU, Department of Physics, Peking University , PETER A. DOWBEN, Department of Physics, University of Nebraska -Lincoln, DEPARTMENT OF PHYSICS, UNIVERSITY OF NEBRASKA AT OMAHA COLLABORATION, DEPARTMENT OF PHYSICS, PEKING UNIVERSITY COLLABORATION, DEPARTMENT OF PHYSICS, UNIVERSITY OF NEBRASKA-LINCOLN COLLABORATION — We used on-site correlation corrected density functional theory to investigate the structure and magnetic properties of the recently synthesized B_5CX-Co and many other substitutions. We found that the Co and Ni molecules were non-magnetic. Other than that: Cr had both stable ferro- and antiferromagnetic structures. The V, Mn, and Fe molecules are not stable, we have to treat them as infinitely long chain molecules.

Dayne Shields
Physics Department of University of Nebraska at Omaha

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