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IMPROVING THE STABILITY AND MAGNETIC HARDENING OF FE16N2 BY ALLOYING: A FIRST-PRINCIPLES STUDY

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Fe16N2, a promising alternative to rare-earth based permanent magnets, has a very limited applicability due to its poor thermal stability. In this work, using density functional theory method, we investigate the e ect of alloying Fe16N2 with 3d and 4d transition group elements on its formation energy and magnetic properties. Using a systematic screening procedure, we propose Vanadium (V) as an excellent alloying element that improves both the stability and magneto-crystalline anisotropy energy (MAE) of Fe16N2. Our work demonstrates that alloying Fe16N2 with V improves its MAE by 20% in addition to making it suitable for high temperature applications. Synergistic improvement in both these performance parameters has not been reported so far. Our work provides useful inputs for experimental e orts to stabilize Fe16N2.

BIOGRAPHY

Satadeep Bhattacharjee holds a PhD degree in physics and has expertise in the broad area of materials theory. Prior to joining the IKST, he worked in different places such as University of Bonn (Germany), University of Liege (Belgium), Uppsala University (Sweden), RIKEN (Japan) and University of Arkansas in USA. He has authored 20+ research papers in reputed journals. Satadeep has worked in different areas such as electronic structure of low dimensional correlated systems, multiferroics, magnetic multilayers, magnetic molecules, magnetic memory materials etc. His current research interest involves heterogeneous catalysis.

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