

Two-dimensional multiferroicity and half-metallicity of the carrier-doped 2H-VSiN₃ monolayer

Long Gong¹, Ming-Yang Liu^{2*}, Yao He¹, and Kai Xiong³

¹*Department of Physics, Yunnan University, Kunming 650091, P. R. China*

²*School of Physics & Electrical and Energy Engineering, Chuxiong Normal University, Chuxiong 675000, P. R. China*

³*Materials Genome Institute, School of Materials and Energy, Yunnan University, Kunming 650091, P. R. China*

Corresponding author: Ming-Yang Liu (E-mail: 18788549890@163.com)

1. The POSCAR of 2H-VSiN₃

VSi2N4

1.0000000000000000

2.8800001144000000 0.0000000000000000 0.0000000000000000

-1.4400000572000000 2.4941532620000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.9575004577999984

V N Si

1 3 1

Direct

0.6315675804203328 0.2922520416124520 0.0644844996529914

0.9649010644684963 0.9589190036362220 0.0325630525281929

0.9649008489870623 0.9589174530599095 0.1071963193654172

0.2982318379329281 0.6255791454365954 0.1831858330424369

0.9648986931911795 0.9589123682548182 0.1655202934109571