Single-layer metal halides MX₂ (X = Cl, Br, I): stability and tunable magnetism from first principles and Monte Carlo simulation

Vadym V. Kulish¹, Wei Huang²

¹Department of Mechanical Engineering, National University of Singapore, 21 Lower Kent Ridge Rd, 119077, Singapore

²Institute of Systems Science, National University of Singapore, 25 Heng Mui Keng Terrace, 119615, Singapore

E-mails: kulishvadym@gmail.com (V.V.K), huangwei860921@gmail.com (W.H)

Electronic supplementary information
Figure S1. Calculated phonon dispersions of single-layer dihalides
Figure S2. Density of states (DOS) of Co, Ni, Fe and Mn-based single-layer dihalides calculated using the HSE functional.
Figure S3. Density of states (DOS) of V and Cr-based single-layer dihalides calculated using the HSE functional