Electronic Supplementary Material (ESI) for RSC Advances.

Antiferromagnetic ordering in the TM-adsorbed AlN monolayer (TM = V and Cr)

Duy Khanh Nguyen[a], Tuan V. Vu[b,c], and D. M. Hoat[d,e,*]

[a]High-Performance Computing Lab (HPC Lab), Information Technology Center, Thu Dau Mot University, Binh Duong Province, Vietnam

[b]Division of Computational Physics, Institute for Computational Science, Ton Duc Thang University, Ho Chi Minh City, Viet Nam

[c]Faculty of Electrical & Electronics Engineering, Ton Duc Thang University, Ho Chi Minh City, Viet Nam

[d]Institute of Theoretical and Applied Research, Duy Tan University, Ha Noi 100000, Viet Nam

[e]Faculty of Natural Sciences, Duy Tan University, Da Nang 550000, Viet Nam

[*]Corresponding author: dominhhoat@duytan.edu.vn

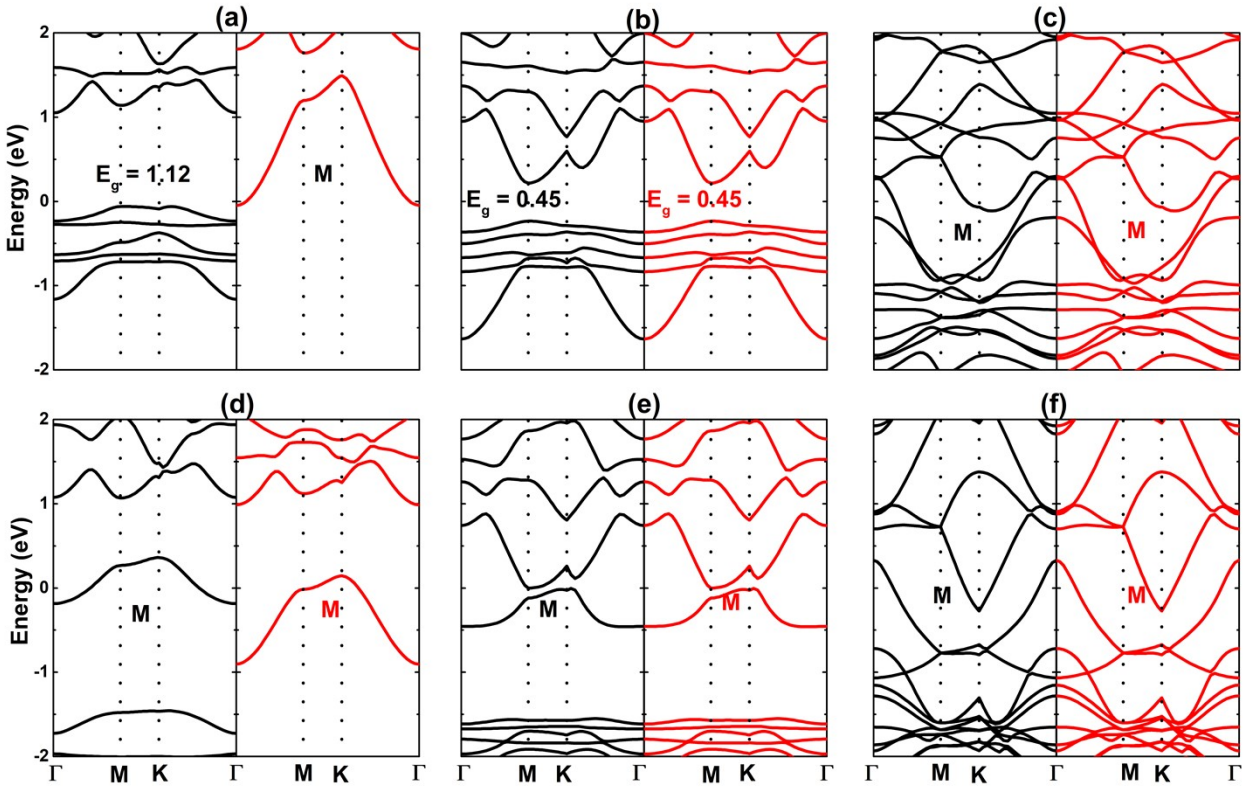

Figure S1: Spin-resolved band structure (Black line: spin-up; Red line: spin-down; E_g: electronic band gap; M: metallic nature) of the V- and Cr-adsorbed AlN monolayer calculated by DFT-D3 with coverage of (a)-(d) 0.25 ML; (b)-(e) 0.5 ML; and (c)-(f) 1.0 ML.

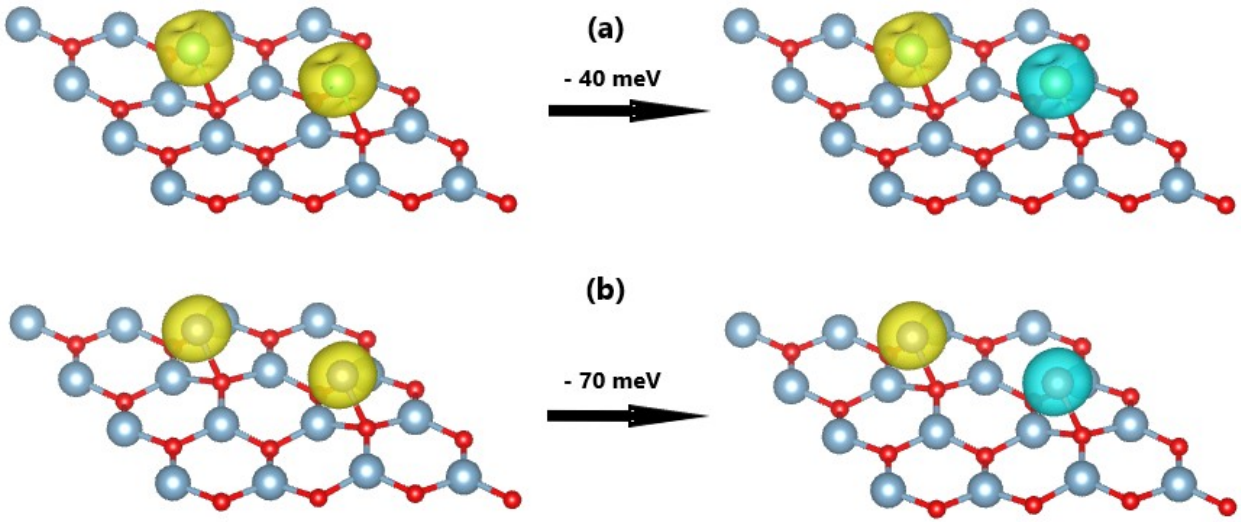

Fig.S2: Energy of magnetic transition of (a) V- and (b) Cr-adsorbed AlN monolayer in a 4×4×1 supercell.

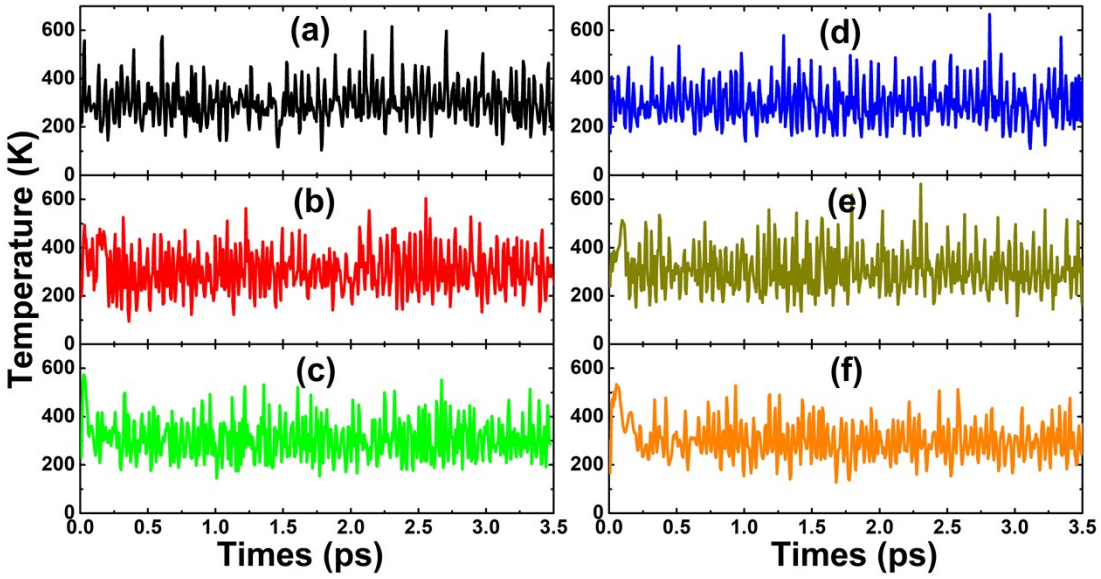

Fig.S3: Fluctuation of temperature as a function of molecular dynamics simulation steps at 300 K of V- and Cr-adsorbed AlN monolayer with coverage of (a-d) 0.25 ML, (b-e) 0.50 ML, and (c-f) 1.0 ML.