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MAGNETISM OF TWO-DIMENSIONAL HAFNENE LAYER

Few years ago, it was claimed that the two-dimensional ferromagnetic planar Hf monolayer could be synthesized on Ir(111). However, many open questions was still remained. Hereby, we unravel the structural stability and its influence on the magnetism using first principles calculations. Despite the ferromagnetic state in planar free-standing Hf layer, extensive systematic calculations with phonon spectra reveal that a planar free-standing Hf layer is unstable and it has a non-magnetic high-buckled structure in ground state. We also find a structural transition from buckled to flat honeycomb geometry on Ir(111) substrate. Nonetheless, the 2D hafnene has no magnetic state due to the strong hybridization with Ir(111) surface. The evolution from non-magnetic to ferromagnetic state incorporated with structural transition is found by adding BN as a spacer layer on Ir(111) substrate (BN/Ir(111)). Besides, we find that the 2D Hf on BN/Ir(111) has a giant perpendicular magnetic anisotropy of 3.41 meV.

References

[1] L. Li, Y. Wang, S. Xie, X.-B. Li, Y.-Q. Wang, R. Wu, H. Sun, S. Zhang and H.-J. Gao, *Nano Lett.*, 2013, **13**, 4671–4674.
[2] Y. Pan, L. Zhang, L. Huang, L. Li, L. Meng, M. Gao, Q. Huan, X. Lin, Y. Wang, S. Du, H.-J. Freund and H.-J. Gao, *Small*, 2014, **10**, 2215–2225.

Figures

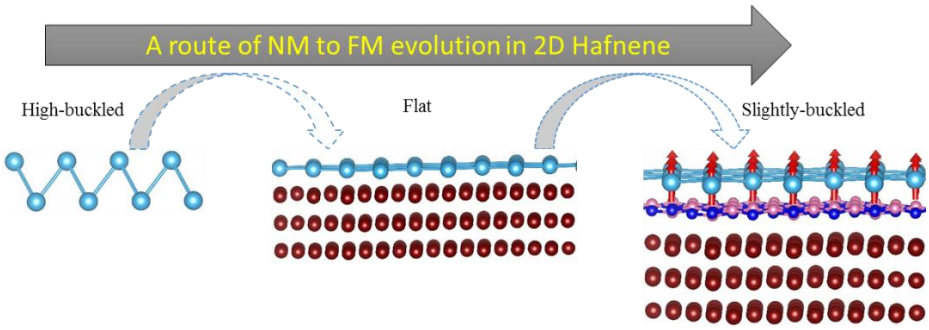

Figure 1: Schematic illustration for a path way for the transition from a non-magnetic state to ferromagnetic state.