Electronic Supplementary Information (ESI)

Theoretical prediction of two-dimensional HfB_2 monolayer with Dirac cone and remarkable Fermi velocity

Zhongfei Liu,[a] Peihong Wang,[a] Qiaoyu Cui,[a] Guang Yang,[b] Shaowei Jin*,[a,c] and Kuangwei Xiong*,[d]

a. School of Physics and Materials Science, Anhui University, Hefei 230601, P. R. China

b. College of Energy and Environmental Engineering, Hebei University of Engineering, Handan 056038, Hebei Province, P. R. China

c. Anhui Key Laboratory of Information Materials and Devices, Hefei 230601, Anhui Province, P. R. China

d. Department of Physics, East China Jiaotong University, Nanchang 330013, Jiangxi Province, P. R. China

Corresponding author

Shaowei Jin: jinsw@mail.ustc.edu.cn

Kuangwei Xiong: 49548967@ecjtu.jx.cn

Computational Details of Benchmarks

The computations with different values of cutoff energies, k-point grid and vacuum thickness were performed to benchmark all the computational model, which could balance the computational precision and computing cost. According to our computations, the first Brillouin zone was sampled with a 9×9×1 Γ-centered Monkhorst-Pack k-point grid, the energy cutoff was set to 600 eV and the vacuum layer was set to larger than 15 Å, which were large enough to reach the requirements.

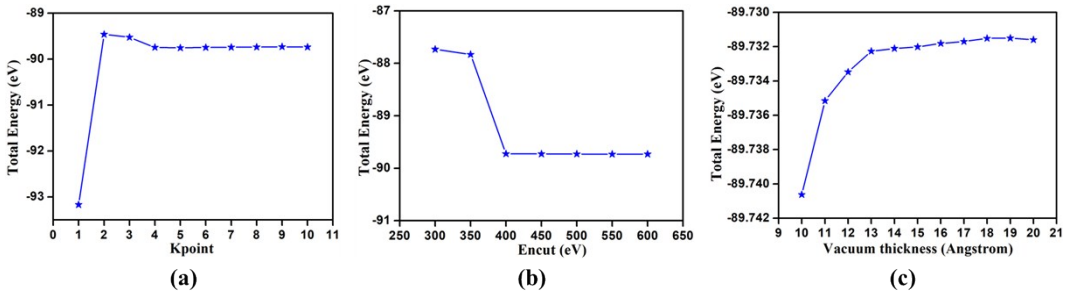

Fig S1 Benchmark computations: the relationship of total energy of the HfB_2 monolayer with (a) k-point (b) energy cutoff (c) vacuum thickness.

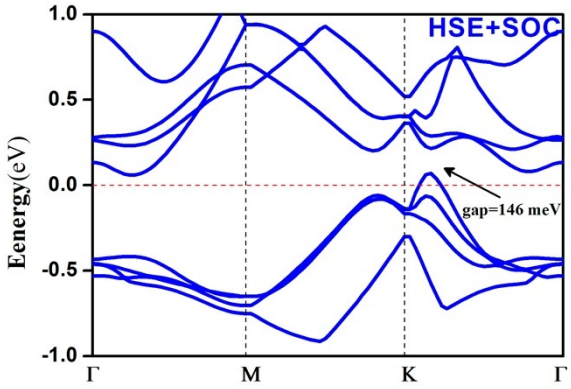

Fig S2 Calculated band structure of HfB_2 monolayer with HSE06 functional method after considering SOC. The red dashed line denotes Fermi level.

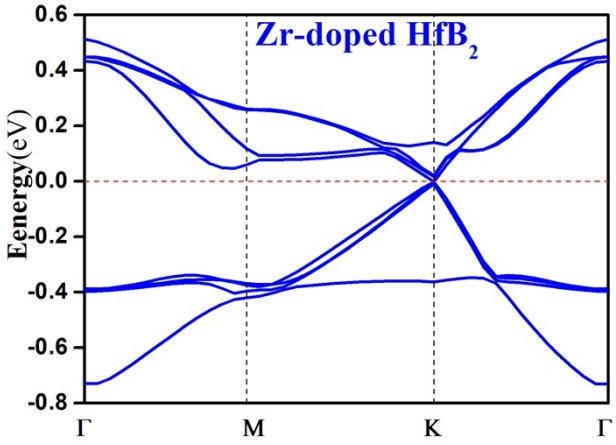

Fig. S3 The band structure of Zr doped HfB_2 monolayer computed by PBE functional.

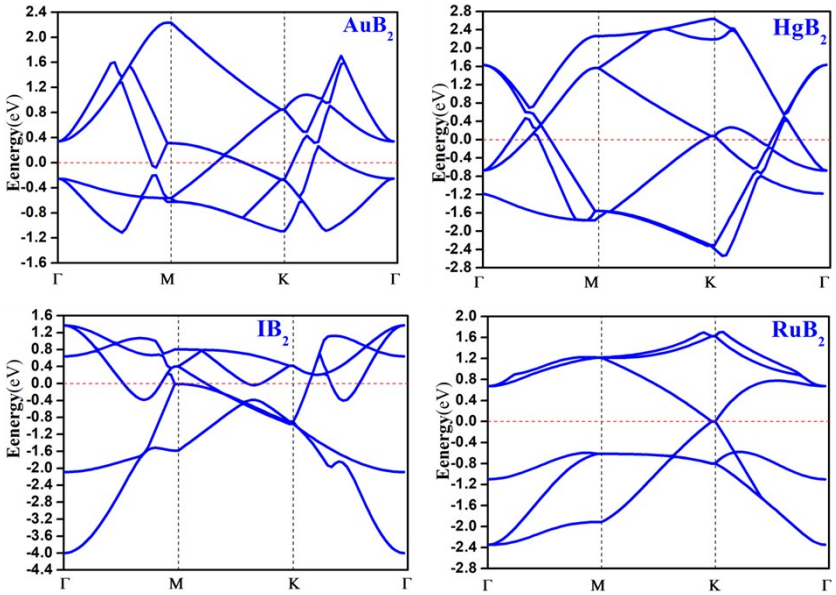

Fig S4 Band structure of some atoms with high enough redox potentials, which combined with B atoms.

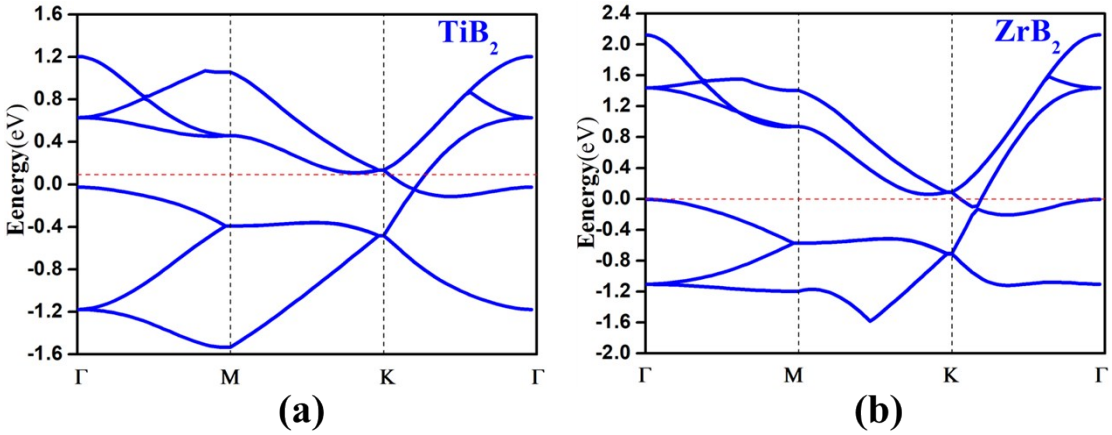

Fig S5 Band structure of the TiB_2 and ZrB_2 monolayer with PBE functional.

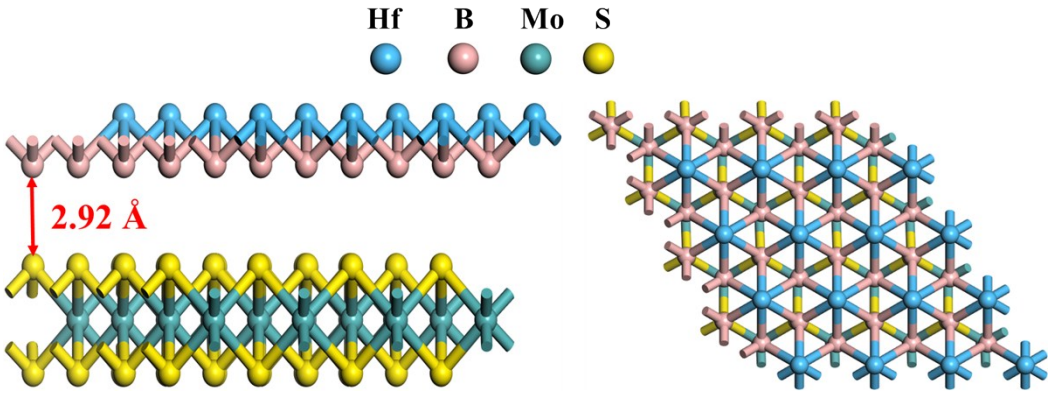

Fig S6 Side and top views of the grown 2D HfB_2 monolayer on MoS_2 substrate

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Hf B
   1.00000000000000
     5.5543436443466971    -3.2068171616009082     0.0000000000000000
    -0.0000133050649470     6.4136112781533301     0.0000000000000000
     0.0000000000000000     0.0000000000000000    23.9522403661646131
   Hf   B
     4     8
Direct
  0.0000000000000000  0.0000000000000000  0.5402746014381026
  0.5000000000000000  0.0000000000000000  0.5402746014381026
  0.0000000000000000  0.5000000000000000  0.5402746014381026
  0.5000000000000000  0.5000000000000000  0.5402746014381026
  0.1666667183406432  0.3333332816593639  0.4816126992809464
  0.6666667183406432  0.3333332816593639  0.4816126992809464
  0.1666667183406432  0.8333332816593639  0.4816126992809464
  0.6666667183406432  0.8333332816593639  0.4816126992809464
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  0.8333332816593639  0.1666667183406361  0.4816126992809464
  0.3333332816593639  0.6666667183406361  0.4816126992809464
  0.8333332816593639  0.6666667183406361  0.4816126992809464
```

Fig S7 Structural parameter of the HfB_2 monolayer in POSCAR file.

Table S1 Cohesive Energies of some atoms with high enough redox potentials, which combined with B atoms. The HfB_2 Dirac material is highlighted in bold

	HfB_2	AuB_2	HgB_2	IB_2	RuB_2
Cohesive energies (eV/atom)	**6.12**	3.07	1.07	0.02	6.46