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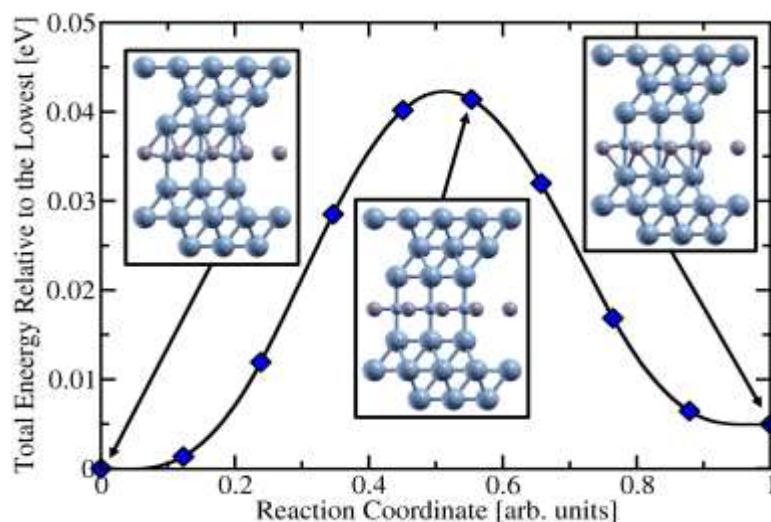
## A Theoretical Estimate of the Energy Barrier between Bi-stable state in Ni/hBN/Ni

We carried out an ab-initio study of hexagonal boron nitride (hBN) sandwiched between Ni(111) layers to understand the properties of the interface in this material structure. The Ni(111)/hBN/Ni(111) structure with Ni slabs consisting of three Ni atomic layers was considered to determine the exact atom arrangement at the interface. The stability of the stacking, as well as the electronic properties, were determined using spin-polarized generalized gradient approximations of density functional theory. The results for 36 stacking arrangements, which are doubled with respect to the magnetic alignment of slabs in an anti-parallel configuration (APC) and parallel configuration (PC), revealed that the number of formed weak chemical bonds, in the pd-hybridization between the N and Ni atoms, is decisive. A maximum of two pd-hybridization bonds stabilized the structure, with APC proving to be the most favorable magnetic alignment, in line with the results of previous experimental studies [1]. In the lowest energy state, an induced magnetic moment at an N site appears when N is moved closer to one of the Ni atoms. Interestingly, the moment direction is switched by the position of the N layer in the resulting bi-stable state with electrical polarization when APC is chosen [2]. Nudged Elastic Band (NEB) calculation has been done to obtain the energy required to switch between the two bi-stable states. Our result show that the small energy barrier is estimated  $\approx 42$  meV as shown in Fig 1. Further investigation is still needed to understand comprehensively the switching mechanism in this Ni/hBN/Ni system.

### References

- [1] M. Z. Iqbal et. al., Adv. Eng. Mater., (2018) 20,1700692
- [2] H. Harfah et. al., arXiv:1905.12252

### Figures



**Figure 1:** NEB calculation result of bi-stable state in Ni/hBN/Ni.