

Electronic Supplementary Information

High magnetoresistance of hexagonal boron nitride- graphene heterostructure-based MTJ through excited-electron transmission

Halimah Harfah,^{*a‡} Yusuf Wicaksono,^{a‡} Gagus Ketut Sunnardianto,^c Muhammad Aziz Majidi,^b and Koichi Kusakabe^{a,d}

a. Graduate School of Engineering Science, Osaka University, 1-3 Machikaneyama-cho, Toyonaka, Osaka 560-8531, Japan.

b. Department of Physics, Faculty of Mathematics and Natural Science, Universitas Indonesia, Kampus UI Depok, Depok, Jawa Barat 16424, Indonesia.

c. Research Center for Physics, The National Research and Innovation Agency, Kawasan Puspiptek Serpong, Tangerang Selatan, 15314, Banten, Indonesia.

d. School of Science, Graduate School of Science, University of Hyogo, 3-2-1 Kouto, Kamigori-cho, Ako-gun, Hyogo, 678-1297, Japan.

[‡] These authors contributed equally to this work

* Corresponding author; E-mail: harfah.h@opt.mp.es.osaka-u.ac.jp

Table S1. The comparison between various van der Waals interactions method in DFT calculation on Ni/3hBN/Ni MTJ respect to experimental result on epitaxial hBN placed on Ni(111) surface [1] and bulk hBN [2]. DFT-D3 and DFT-D2 show an interlayer distance between Ni-hBN and hBN-hBN closer to experimental values.

	Ni-hBN Layer Distance	hBN-hBN layer Distance
Experimental	$1.87 \pm 0.12 \text{ \AA}$ [1]	3.33 \AA [2]
DFT-D2 method	2.07 \AA (N-Ni)	3.44 \AA (N-B)
	1.95 \AA (B-Ni)	3.56 \AA (B-N)
DFT-D3 method	2.05 \AA (N-Ni)	3.13 \AA (N-B)
	1.93 \AA (B-Ni)	3.25 \AA (B-N)
vdW-DF method	3.52 \AA (N-Ni)	3.53 \AA (N-B & B-N)
	3.52 \AA (B-Ni)	
vdW-DF2 method	3.56 \AA (N-Ni)	3.48 \AA (N-B & B-N)
	3.56 \AA (B-Ni)	

[1] Tonkikh, A. A. et. al., Structural and electronic properties of epitaxial multilayer h-BN on Ni(111) for spintronics applications. *Sci. Rep.* **6**, 23547 (2016).

[2] Lynch, R. W. Effect of high pressure on the lattice parameters of diamond, graphite, and hexagonal boron nitride. *J. Chem. Phys.* **44**, 181 (1966).

Figure S1. The transmission probability of Ni/3hBN/Ni and Ni/hBN-vacuum-hBN/Ni in PC state for spin-up and spin-down electrons. The hBN at the interfaces distance of Ni/hBN-vacuum-hBN/Ni MTJ was made same with Ni/3hBN/Ni MTJ. This result shows that the wide-gap insulator of hBN can never be treated as a vacuum for the conducting electron. This result also indicates that the high transmission probability peak of the spin-down electron in the PC state found in the 3hBN, 4hBN, and 5hBN system comes from the proximity effect, which works on middle hBN.

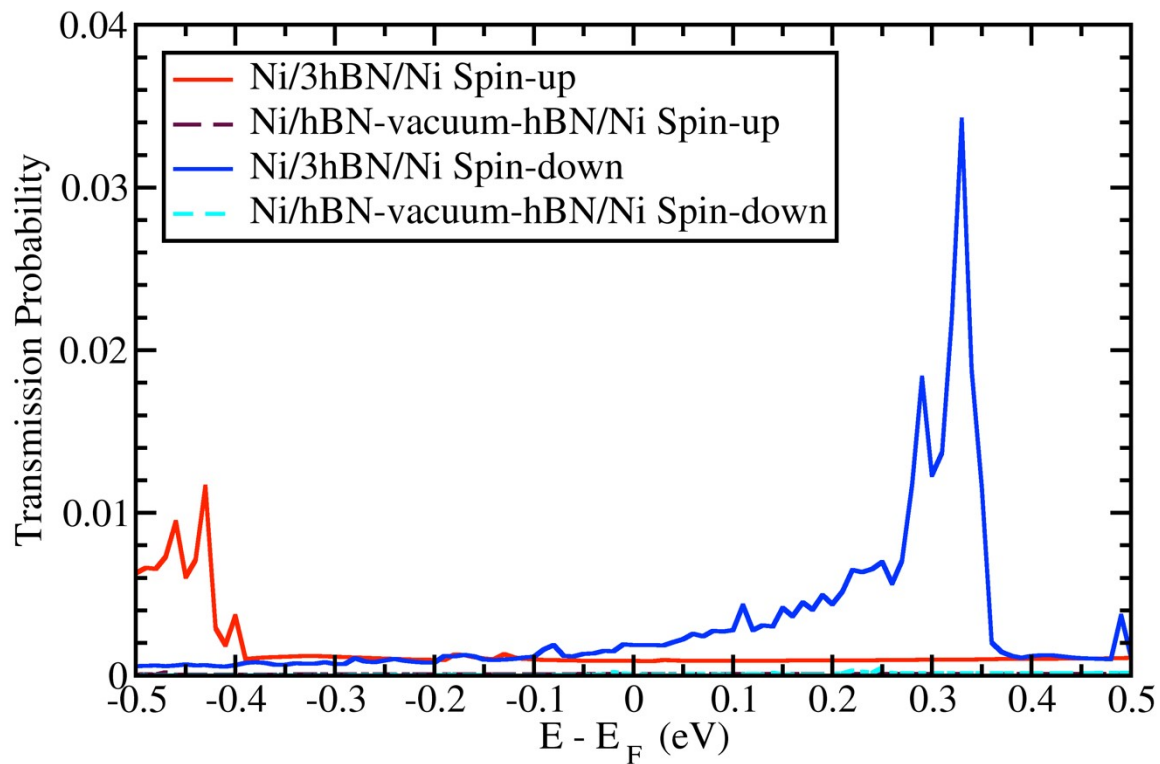


Figure S2. The local density of states (LDOS) of insulator barrier of (a) Ni/3hBN/Ni and (b) Ni4hBNNi (only middle hBN shows in the graph) when upper and lower Ni slabs in anti-parallel configuration (APC).

