## Supporting Information for: First principle study of electronic transport properties in novel FeB<sub>2</sub> flakes-based nanodevices

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Figure S1 (a)-(j) Equilibrium transmission spectra of devices  $M_{opti}$ ,  $M_{300K}$ ,  $M_{500K}$ ,  $M_{600K}$ ,  $M_{800K}$ ,  $M_{1000K}$ ,  $M_{1200K}$ ,  $M_{1500K}$ ,  $M_{1800K}$  and  $M_{2000K}$  in the energy range [-3eV, 3eV] respectively.

Energy	= 0.000000e+00 eV
Number of transmission	n modes = 26
Eigenvalues (Up):	+
8.747147e-01	
1.622041e-01	
3.166149e-03	
3.498321e-04	
3.166171e-05	
1.715802e-05	
7.039644e-07	
1.463359e-07	
7.769243e-10	
6.783836e-12	
9.282031e-14	
2.696723e-14	
7.134395e-15	
5.034369e-15	
3.428690e-15	
6.923854e-16	
2.705431e-16	
9.651231e-17	
5.479017e-17	
4.286182e-17	
2.858477e-17	
1.426340e-17	
9.995142e-18	
6.517246e-18	
8.188708e-19	
3.230537e-19	
+	+

Figure S2 Transmission eigenvalues report of device  $M_{300K}$  at the Fermi level.



**Figure S3** (a)-(f) Structures of devices with 3, 4, 5, 6, 7, 8-atoms wide flakes with the same edge atom arrangement. (g) Transmission spectra of these devices around the Fermi level.



Figure S4 (a)-(f) Transmission pathways of representative  $FeB_2$  devices (devices  $M_{opti}$ ,  $M_{300K}$ ,  $M_{500K}$ ,  $M_{1000K}$ ,  $M_{1500K}$  and  $M_{2000K}$ , respectively).