Supporting Information

Strain Controlled Ferromagnetic-Antiferromagnetic Transformation in Mn-Doped Silicene for Information Transformation Devices

Shuang Li,[1] Zhimin Ao,[2] Jiaji Zhu,[3] Jichang Ren,[4] Jiabao Yi,[5] Guoxiu Wang,[6] and Wei Liu[1]*

[1]Nano Structural Materials Center, School of Materials Science and Engineering, Nanjing University of Science and Technology, Nanjing 210094, Jiangsu, China

*Email: weiliu@njust.edu.cn

[2]School of Environmental Science and Engineering, Guangdong University of Technology, Guangzhou 510006, China

[3]Institute for Quantum Information and Spintronics, School of Science, Chongqing University of Posts and Telecommunications, Chongqing 400065, China

[4]Physics Department, National University of Singapore, 2 Science Drive 3, Singapore 117551, Republic of Singapore

[5]School of Materials Science and Engineering, University of New South Wales, Sydney 2052, NSW, Australia

[6]Centre for Clean Energy Technology, School of Mathematical and Physical Sciences, University of Technology Sydney, PO Box 123, Broadway, Sydney, NSW 2007, Australia

Figure S1. Top view and side view for optimized configurations of TMA adsorbed on (a) hollow position of the pristine silicene, (b) bridge position of pristine silicene, and (c) SV and (d) DV in silicene. Gray and yellow spheres denote the TMA and the silicon atom, respectively.

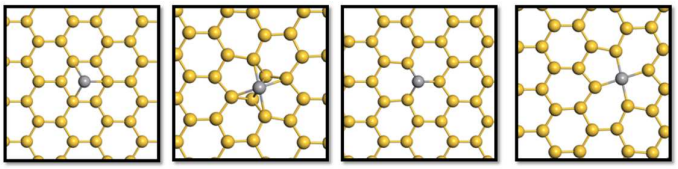

Figure S2. (a) Metal-silicon bond lengths, (b) the elevation of the TMAs above the silicene surface, and (c) binding energies E_b for TMAs on silicene. Blue, red and green curves denote TM@P-Si, TM@SV and TM@DV systems, respectively. The elevation h is defined as the vertical distance between TM atoms and the down layer silicon atoms. The binding energy of TMA decorated silicene can be defined as: $E_b=E_{tot}$ - $E_{Silicene}$ - E_{TM}, where E_{tot} is the total energy of the optimized system (the systems are TMA adsorbing on silicene or TMA embedding in silicene with vacancies), $E_{Silicene}$ is the total energy of silicene without and with vacancy, E_{TM} is the energy of an isolated TM atoms in the gas phase.

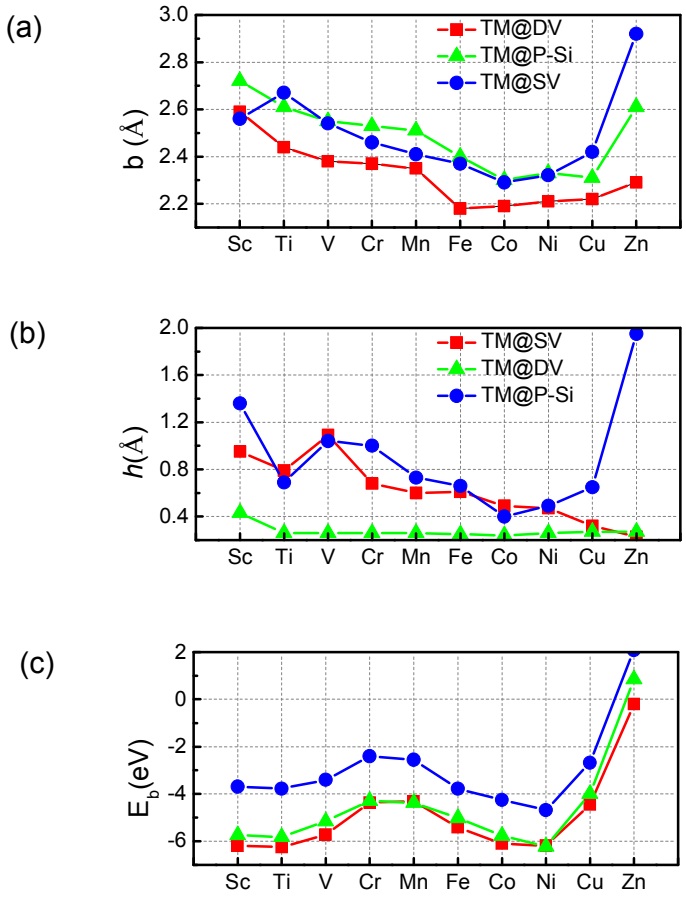

Figure S3. Computed magnetic moments of the Mn@SV system and the Mn dopants as a function of *U* values.

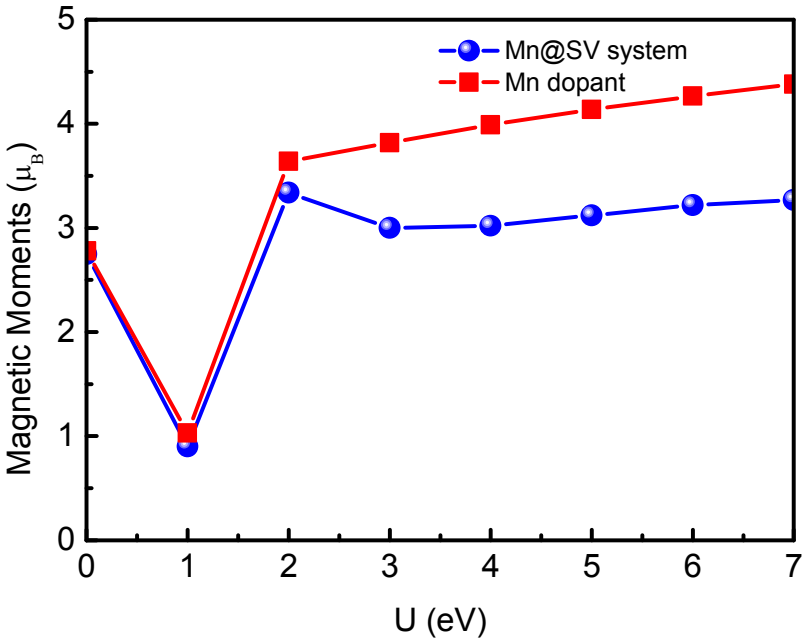

Table SI Calculated magnetic moments by using HSE for TM@P-Si, TM@SV, and TM@DV. μ_{Tot}, μ_{TM}, and $\mu_{TM\text{-}3d}$ denote the total magnetic moment of the systems, the magnetic moment of TM dopants, and magnetic moment of 3*d* orbital of TM dopants, respectively.

TM@P-Si	μ_{Tot} (μ_B)	μ_{TM} (μ_B)	$\mu_{TM\text{-}3d}$ (μ_B)
Sc	0.98	0.34	0.30
Ti	2.04	1.89	1.78
V	4.99	3.83	3.61
Cr	4.43	4.54	4.27
Mn	3.03	4.14	3.91
Fe	0.78	1.02	0.97
Co	0.00	0.00	0.00
Ni	0.00	0.00	0.00
Cu	0.00	0.00	0.00
Zn	0.00	0.00	0.00
TM@SV	μ_{Tot} (μ_B)	μ_{TM} (μ_B)	$\mu_{TM\text{-}3d}$ (μ_B)
Sc	0.00	0.00	0.00
Ti	0.00	0.00	0.00
V	2.14	2.85	2.78
Cr	2.14	3.80	3.68
Mn	3.51	4.37	4.11
Fe	0.73	2.09	2.00
Co	1.67	1.93	1.75
Ni	2.54	1.22	1.05
Cu	0.37	0.00	0.00
Zn	0.23	0.00	0.0
TM@DV	μ_{Tot} (μ_B)	μ_{TM} (μ_B)	$\mu_{TM\text{-}3d}$ (μ_B)
Sc	0.00	0.00	0.00
Ti	2.61	1.99	1.81
V	2.00	3.00	2.79
Cr	3.05	4.26	3.98
Mn	3.35	4.42	4.13
Fe	0.00	0.00	0.00
Co	1.17	1.39	1.29
Ni	0.00	0.00	0.00
Cu	0.00	0.00	0.00
Zn	0.67	0.00	0.00