Supporting Information for Anisotropic Rashba splitting in Pt-based Janus monolayers PtXY (X,Y = S, Se, or Te)

Paul Albert L. Sino¹, Liang-Ying Feng¹, Rovi Angelo B. Villaos¹, Harvey N. Cruzado^{1,2}, Zhi-Quan Huang¹, Chia-Hsiu Hsu¹, and Feng-Chuan Chuang^{1,3,4}*

¹Department of Physics, National Sun Yat-sen University, Kaohsiung, 80424 Taiwan

²Institute of Mathematical Sciences and Physics, College of Arts and Sciences, University of the Philippines Los Baños, College, Laguna, 4031 Philippines

³Department of Physics, National Tsing Hua University, Hsinchu, 30013 Taiwan

⁴Physics Division, National Center for Theoretical Sciences, Taipei, 10617 Taiwan

*Corresponding Author: Feng-Chuan Chuang

Postal Address: 70 Lienhai Rd., Kaohsiung 80424, Taiwan.

Telephone: +886-7-5253733 E-mail Address: <u>fchuang@mail.nsysu.edu.tw</u>

Material	Туре	$\alpha (\mathrm{eV} \cdot \mathrm{\AA})$	Type of Splitting	Reference
MoS ₂ /Bi (111)	Heterostructure	1.05	Rashba	[1]
Pb Thin Film	Metal Thin Film	0.04	Rashba	[2]
PtBi ₂	Bulk	4.36	Rashba + Dresselhaus	[3]
MoSSe	ML Janus TMD	2.0x10 ⁻³ -1.2	Rashba	[3-5]
WSSe	ML Janus TMD	<1.0	Rashba	[3],[4],[6]
PtSSe	ML Janus TMD	1.65 [*] , 1.33 [†]	Rashba + Dresselhaus	This Work
PtSTe	ML Janus TMD	$1.10^*, 1.24^\dagger$	Rashba + Dresselhaus	
PtSeTe	ML Janus TMD	$0.44^{*}, 0.75^{\dagger}$	Rashba + Dresselhaus	

Table S1. Comparison of the Rashba parameter of Janus PtXY monolayers with well-knownRashba materials.

* α at M- Γ direction, [†] α at M-K direction

- 1. K. Lee, W. S. Yun and J. D. Lee, *Phys. Rev. B*, 2015, **91**, 125420.
- 2. J. H. Dil, F. Meier, J. Lobo-Checa, L. Patthey, G. Bihlmayer, and J. Osterwalder, *Phys. Rev. Lett.*, 2008, **101**, 266802.
- 3. J. Chen, K. Wu, H. Ma, W. Hu and J. Yang, RSC Advances, 2020, 10, 6388–6394.
- 4. Y. C. Cheng, Z. Y. Zhu, M. Tahir and U. Schwingenschlögl, *EPL*, 2013, **102**, 57001.
- 5. F. Li, W. Wei, H. Wang, B. Huang, Y. Dai and T. Jacob, *J. Phys. Chem. Lett.*, 2019, **10**, 559–565.
- 6. W. Zhou, J. Chen, Z. Yang, J. Liu and F. Ouyang, *Phys. Rev. B*, 2019, **99**, 075160.





Figure S1. Band structures under spin-orbit coupling (SOC) of monolayer Janus PtSSe under varying strain from -3.0% to 5.0%. The red and blue colored bands correspond to the valence band maximum (VBM) and conduction band minimum (CBM).





Figure S2. Band structures under SOC of monolayer Janus PtSTe under varying strain from -3.0% to 5.0%. The red and blue colored bands correspond to the VBM and CBM.





Figure S3. Band structures under SOC of monolayer Janus PtSeTe under varying strain from -3.0% to 5.0%. The red and blue colored bands correspond to the VBM and CBM.

K

ΓГ

М

K

Г

Μ

ΓГ

K

-3 ∟ Γ

Μ