Supplementary information: Emergent Wigner phases in moiré superlattice from deep learning

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Supplementary Note 1. Hyperparameters for simulations

The recommended hyperparameters are listed in Supplementary Table 1.

Supplementary Table 1 | Recommended hyperparameters

Hyperparameter	Value	Hyperparameter	Value
Dimension of one electron layer **V**	256	Dimension of two electron layer **W**	32
Number of layers	4	Number of determinants	8
Optimizer	KFAC	Learning rate	1e-2
Damping	1e-3	Constrained norm of gradient	1e-3
Momentum of optimizer	0.0	Batch size	4096
Number of training steps	5e4	Clipping window of gradient	5
MCMC burn in	1e3	MCMC steps between each iterations	30
MCMC move width	2e-2	Target MCMC acceptance	55%
Precision	Float32	Number of inference steps	1e4

Supplementary Note 2. Parameter of moiré potential

Employed model parameters of WSe_2/WS_2 and 2H WS_2 are taken from Refs. [1, 2] and listed in Supplementary Table 2.

Supplementary Table 2 | Model parameters of WSe_2/WS_2 **and** 2H WS_2 .

Systems	V / meV	m^*/m_e	ϕ	ϵ
WSe_2/WS_2	15	0.5	45°	5
2H WS_2	10.3	0.9	20°	5

Model of 3R WS_2 has a slightly different form and its parameters are listed in Supplementary Table 3 [3].

Supplementary Table 3 | Model parameters of 3R WS_2

Systems	V_1 / meV	V_2 / meV	V_3 / meV	m^*/m_e	ϕ	ϵ
3R WS_2	33.5	4.0	5.5	0.87	180°	5

Supplementary Note 3. Calculated energy and geometry

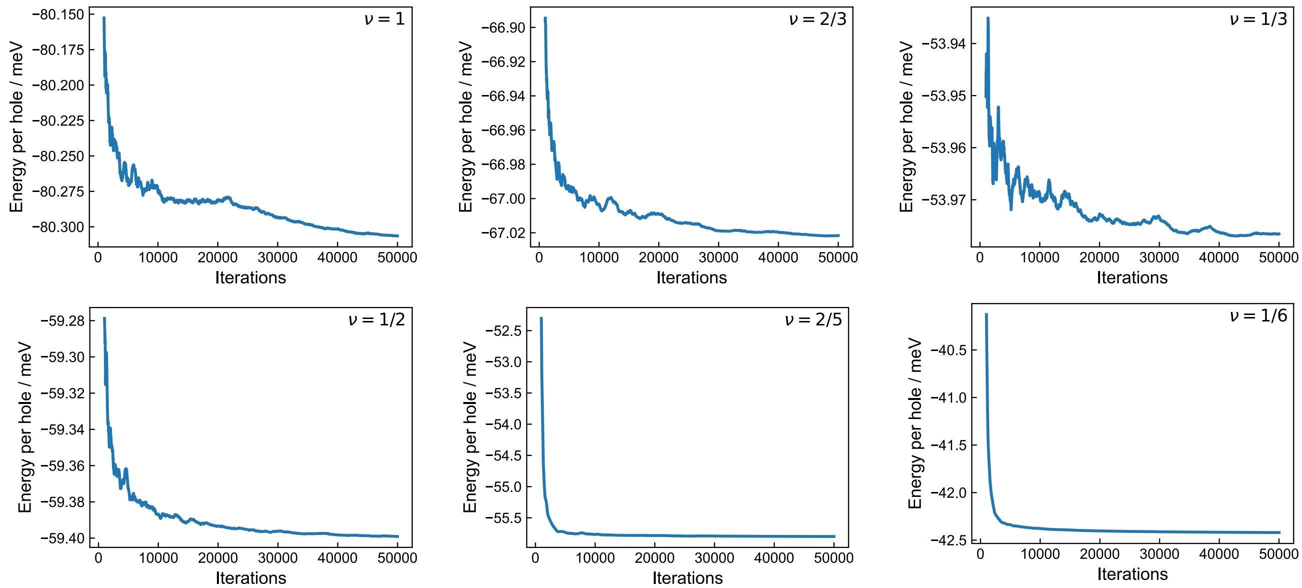
Calculated energies and geometry of each system are listed in Supplementary Table 4.

Supplementary Table 4 | Calculated energies and geometry of each system

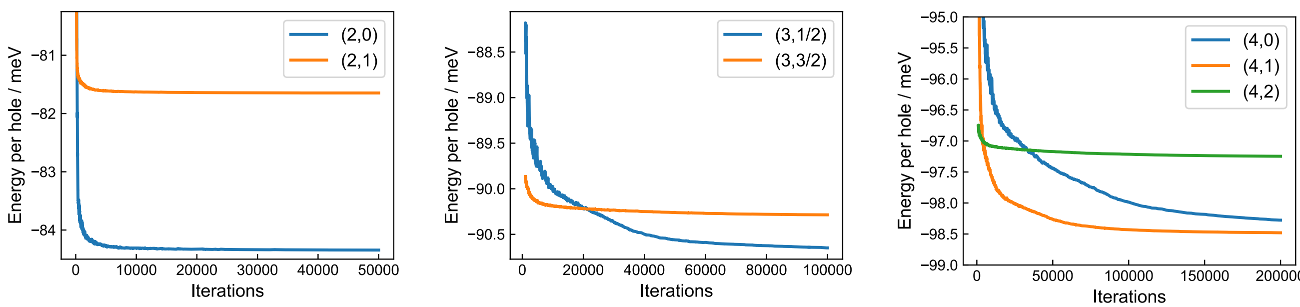
Systems	a_M / nm	fillings ν	S_z	energy per hole / meV	lattice vectors / a_M	supercell size
WSe_2/WS_2	8.3	1	1	-80.2965(2)	$a_1=(1,0),\ a_2=(1/2,\sqrt{3}/2)$	5×5
		2/3	1	-67.0221(1)	$a_1=(3/2,\sqrt{3}/2),\ a_2=(-3/2,\sqrt{3}/2)$	4×4
		1/3	1/2	-53.97697(9)	$a_1=(3/2,\sqrt{3}/2),\ a_2=(-3/2,\sqrt{3}/2)$	5×5
		1/2	1	-59.39885(9)	$a_1=(2,0),\ a_2=(1,\sqrt{3})$	4×4
		2/5	5	-55.7933(2)	$a_1=(5,0),\ a_2=(5/2,5\sqrt{3}/2)$	2×2
		1/6	3	-42.41933(9)	$a_1=(6,0),\ a_2=(3,3\sqrt{3})$	2×2
2H WS_2	9.8	2	0	-84.3421(2)	$a_1=(1,0),\ a_2=(1/2,\sqrt{3}/2)$	3×3
		2	1	-81.64466(7)		
2H WS_2	9.8	3	1/2	-90.6866(2)	$a_1=(1,0),\ a_2=(1/2,\sqrt{3}/2)$	4×4
		3	3/2	-90.2980(1)		
2H WS_2	9.8	4	0	-98.2843(3)	$a_1=(1,0),\ a_2=(1/2,\sqrt{3}/2)$	4×4
		4	1	-98.4657(2)		
		4	2	-97.2430(1)		
3R WS_2	16.51	1	1/2	-102.51681(7)	$a_1=(1,0),\ a_2=(1/2,\sqrt{3}/2)$	3×3
		2	1	-114.6824(2)		
		6	3	-110.5943(2)		
		7	7/2	-110.9851(1)		
		9	9/2	-113.4288(2)		
3R WS_2	16.51	3	1/2	-109.0860(1)	$a_1=(1,0),\ a_2=(1/2,\sqrt{3}/2)$	3×3
		3	3/2	-107.58514(8)		
		4	0	-110.2786(2)		
		4	1	-108.8960(1)		
		4	2	-107.8524(1)		
		5	1/2	-109.5465(1)		
		5	3/2	-109.54138(9)		
		5	5/2	-108.56062(6)		

Supplementary Note 4. Training curves

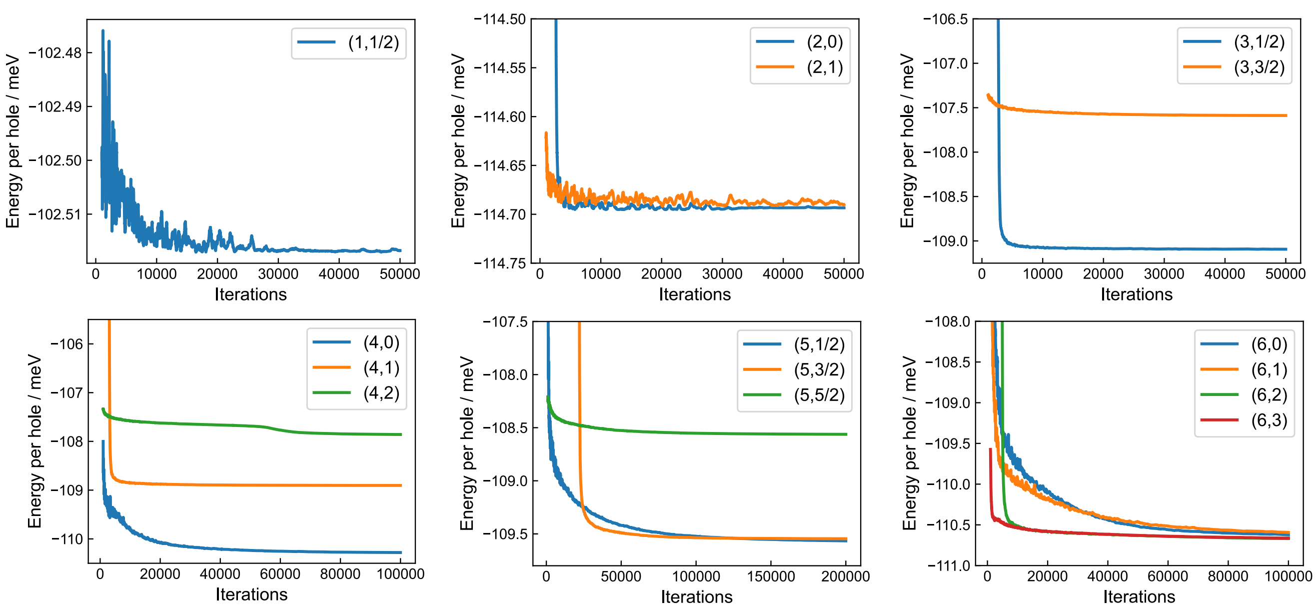
Training curves of each system are plotted in Supplementary Figs. 1 to 3.



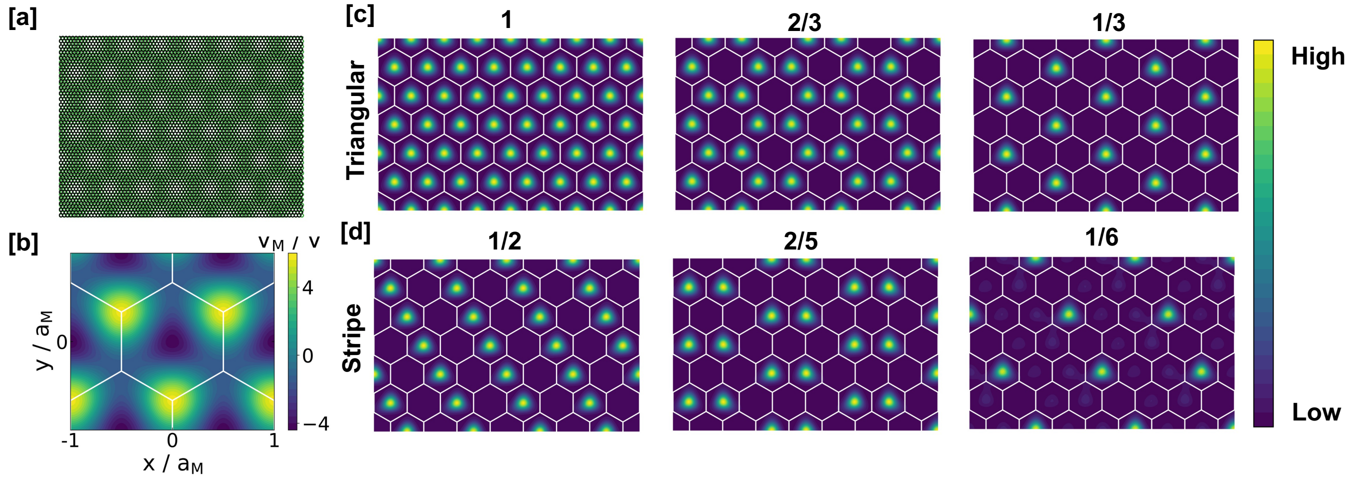
Supplementary Figure 1 | Training curve of various states in WSe_2/WS_2.



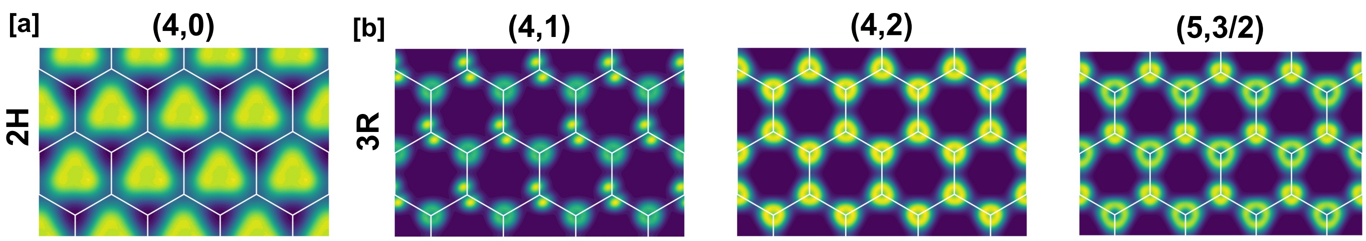
Supplementary Figure 2 | Training curve of various states in 2H WS_2. Tuples in the legends denote the particle fillings and the magnetic number of spin (ν, S_z).



Supplementary Figure 3 | Training curve of various states in 3R WS_2. Tuples in the legends denote the particle fillings and the magnetic number of spin (ν, S_z).



Supplementary Figure 4 | Calculated hole density pattern of WSe_2/WS_2 **heterobilayer**. Numbers above the figures denote the particle fillings ν. **a**, structure of the WSe_2/WS_2 superlattice. **b**, moiré potential of WSe_2/WS_2. a_M denotes corresponding length of moiré cell and is set to 8.3 nm. **c**, calculated triangular phase at fillings $\nu = 1, 2/3, 1/3$. **d**, calculated stripe phase at fillings $\nu = 1/2, 2/5, 1/6$.



Supplementary Figure 5 | Other density patterns of the WS_2 **system**. Tuples above the figure denote the particle fillings and the spin quantum number (ν, S_z). **a-b**, moiré pattern of 2H and 3R WS_2 respectively. All other states with $\nu = 2$ and 6 of the 3R WS_2 system show the same moiré pattern regardless of S_z.

Supplementary Note 5. Other states

Generalized Wigner crystal states and other excited states are plotted in Figs. 4 and 5.

Supplementary References

[1] Hongyuan Li, Ziyu Xiang, Aidan P Reddy, Trithep Devakul, Renee Sailus, Rounak Banerjee, Takashi Taniguchi, Kenji Watanabe, Sefaattin Tongay, Alex Zettl, et al. Wigner molecular crystals from multi-electron moiré' artificial atoms. *arXiv preprint arXiv:2312.07607*, 2023.

[2] Yang Zhang, Noah FQ Yuan, and Liang Fu. Moiré quantum chemistry: charge transfer in transition metal dichalcogenide superlattices. *Physical Review B*, 102(20):201115, 2020.

[3] Mattia Angeli and Allan H MacDonald. γ valley transition metal dichalcogenide moiré bands. *Proceedings of the National Academy of Sciences*, 118(10):e2021826118, 2021.