

# IUCrJ

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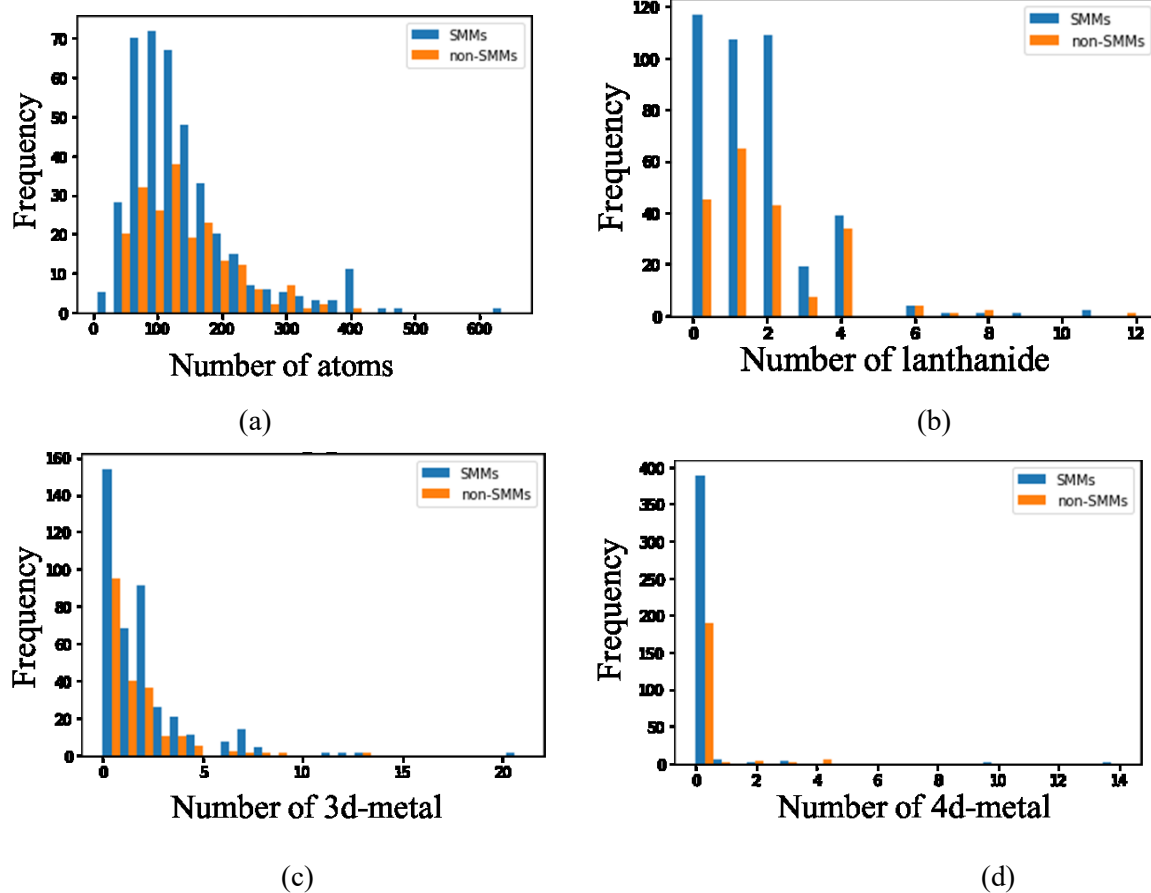
**Supporting information for article:**

**The prediction of single-molecule magnet properties via deep learning**

**Yuji Takiguchi, Daisuke Nakane and Takashiro Akitsu**

**Table S1****Table S2** **Table S1** Detailed information for each layer.

layer name	output size	Layer
conv1	$64 \times 64 \times 64$	$7 \times 7 \times 7, 64$
conv2	$64 \times 64 \times 64$	$\begin{bmatrix} 1 \times 1 \times 1, 16 \\ 3 \times 3 \times 3, 16 \\ 1 \times 1 \times 1, 64 \end{bmatrix} \times 2$
conv3	$32 \times 32 \times 32$	$\begin{bmatrix} 1 \times 1 \times 1, 32 \\ 3 \times 3 \times 3, 32 \\ 1 \times 1 \times 1, 128 \end{bmatrix} \times 2$
conv4	$16 \times 16 \times 16$	$\begin{bmatrix} 1 \times 1 \times 1, 64 \\ 3 \times 3 \times 3, 64 \\ 1 \times 1 \times 1, 256 \end{bmatrix} \times 2$
conv5	$8 \times 8 \times 8$	$\begin{bmatrix} 1 \times 1 \times 1, 128 \\ 3 \times 3 \times 3, 128 \\ 1 \times 1 \times 1, 512 \end{bmatrix} \times 1$
	$1 \times 1 \times 1$	average pool, 1-d fc
Weight		1,153,441



**Figure S1** Figure S1(a) Number of atoms, (b) Number of lanthanide nuclei, (c) Number of 3d metal nuclei, (d) Number of 4d metal nuclei.

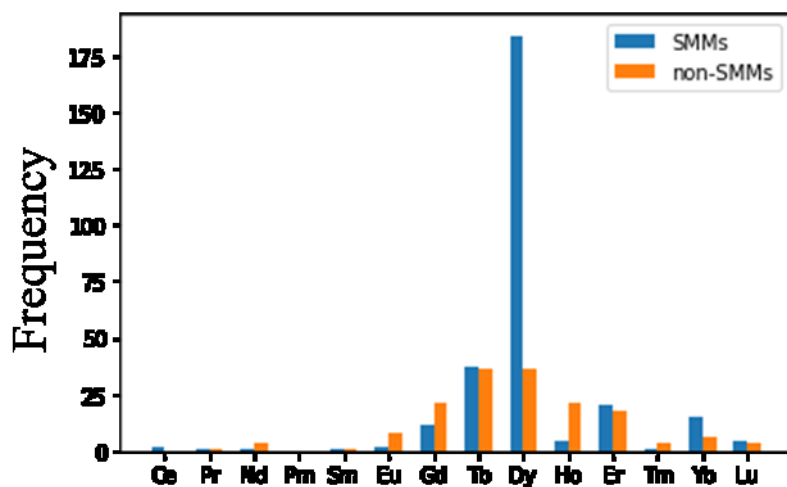
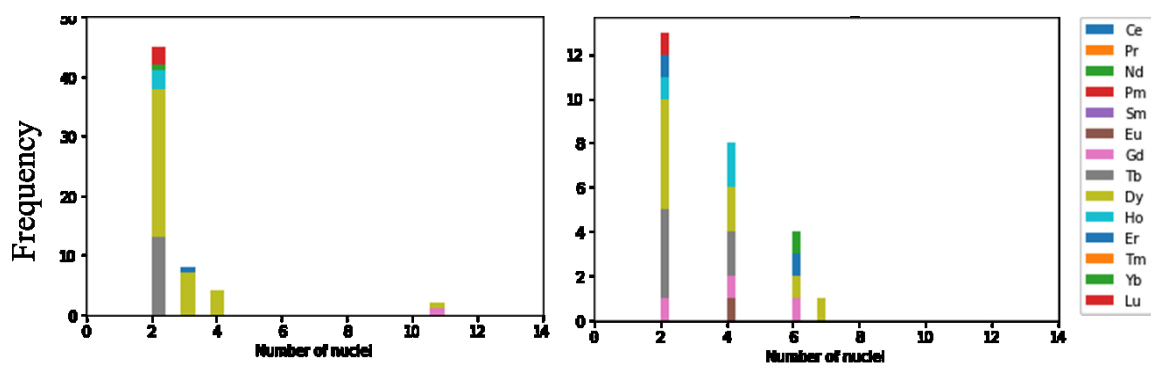


Figure S2 (a)(b)

(c)(d)



(e)

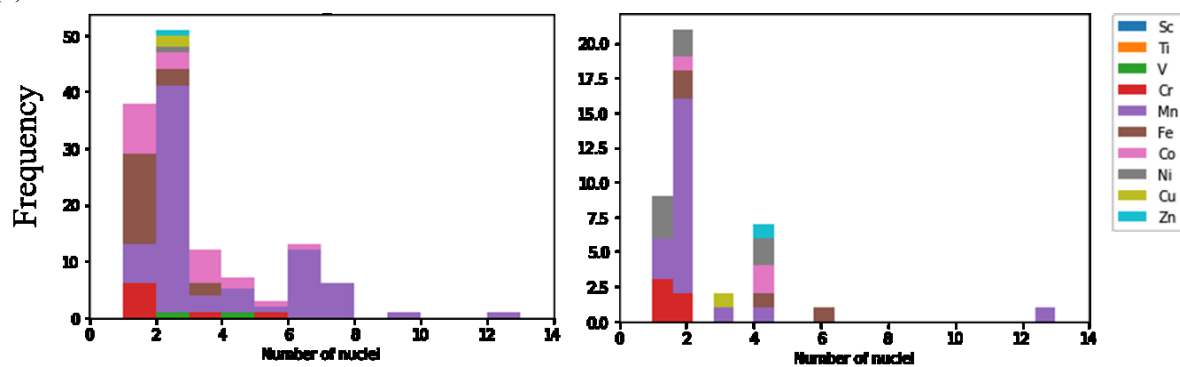


Figure S3 Figure S2(a) Lanthanide ions (b) Number of lanthanide nuclei in SMM molecules, (c)

Number of lanthanide nuclei in non-SMM molecules, (d) Number of d metal nuclei in SMM

molecules, (e) Histogram of the number of d metal nuclei in non-SMM molecules.

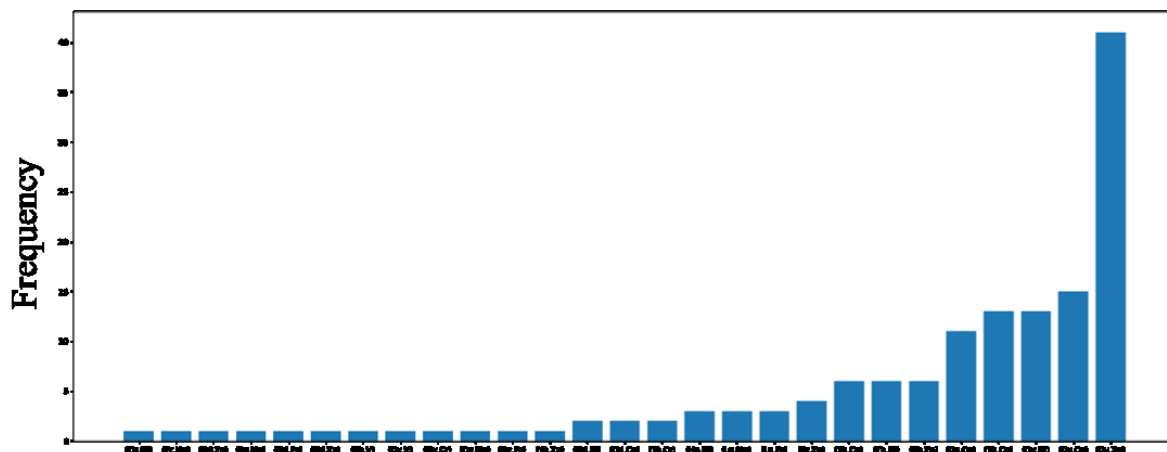


Figure S3 Each 3d-4f metal combinations SMM molecules.

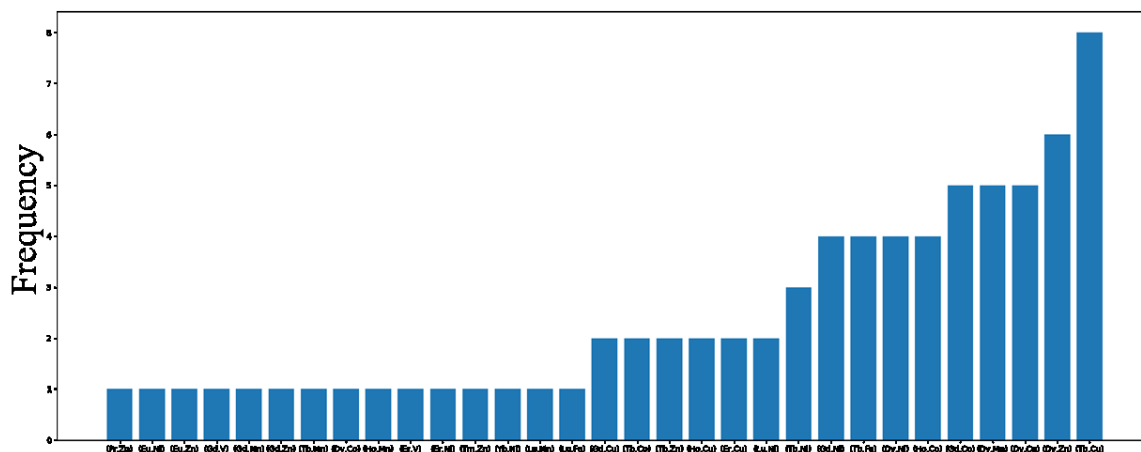
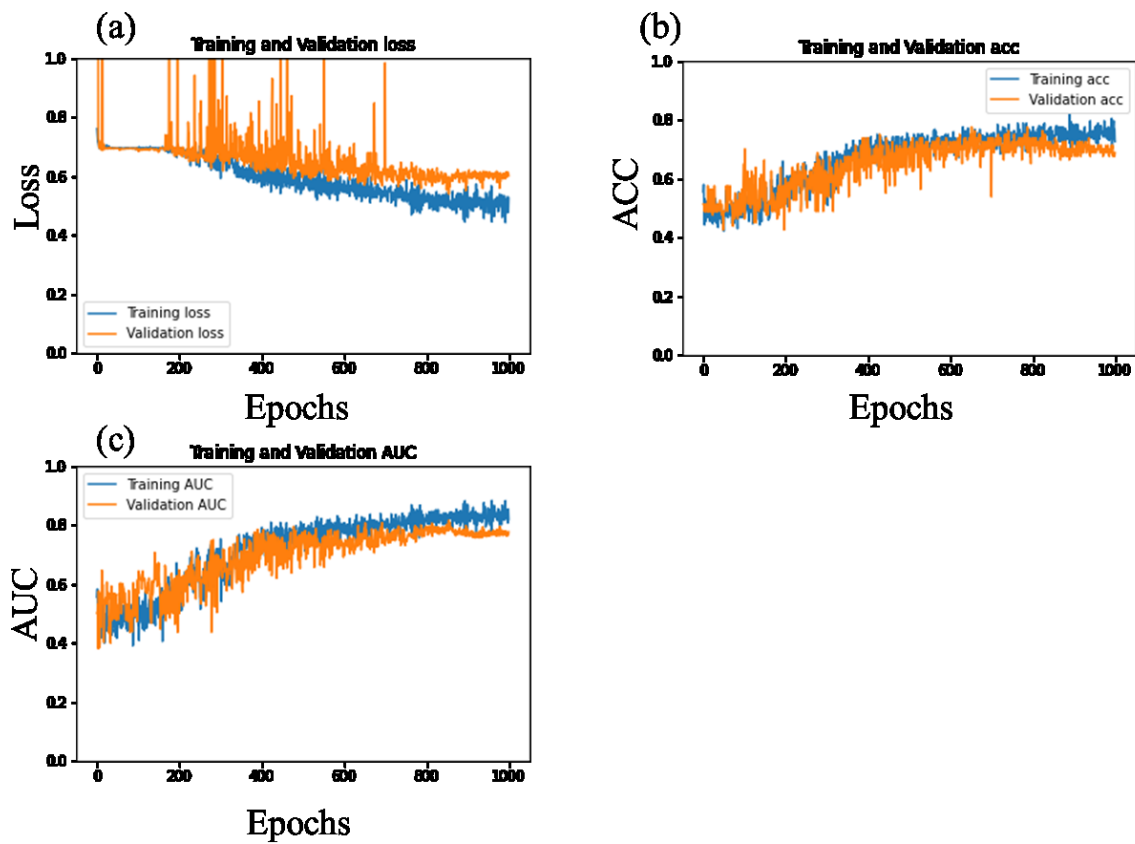
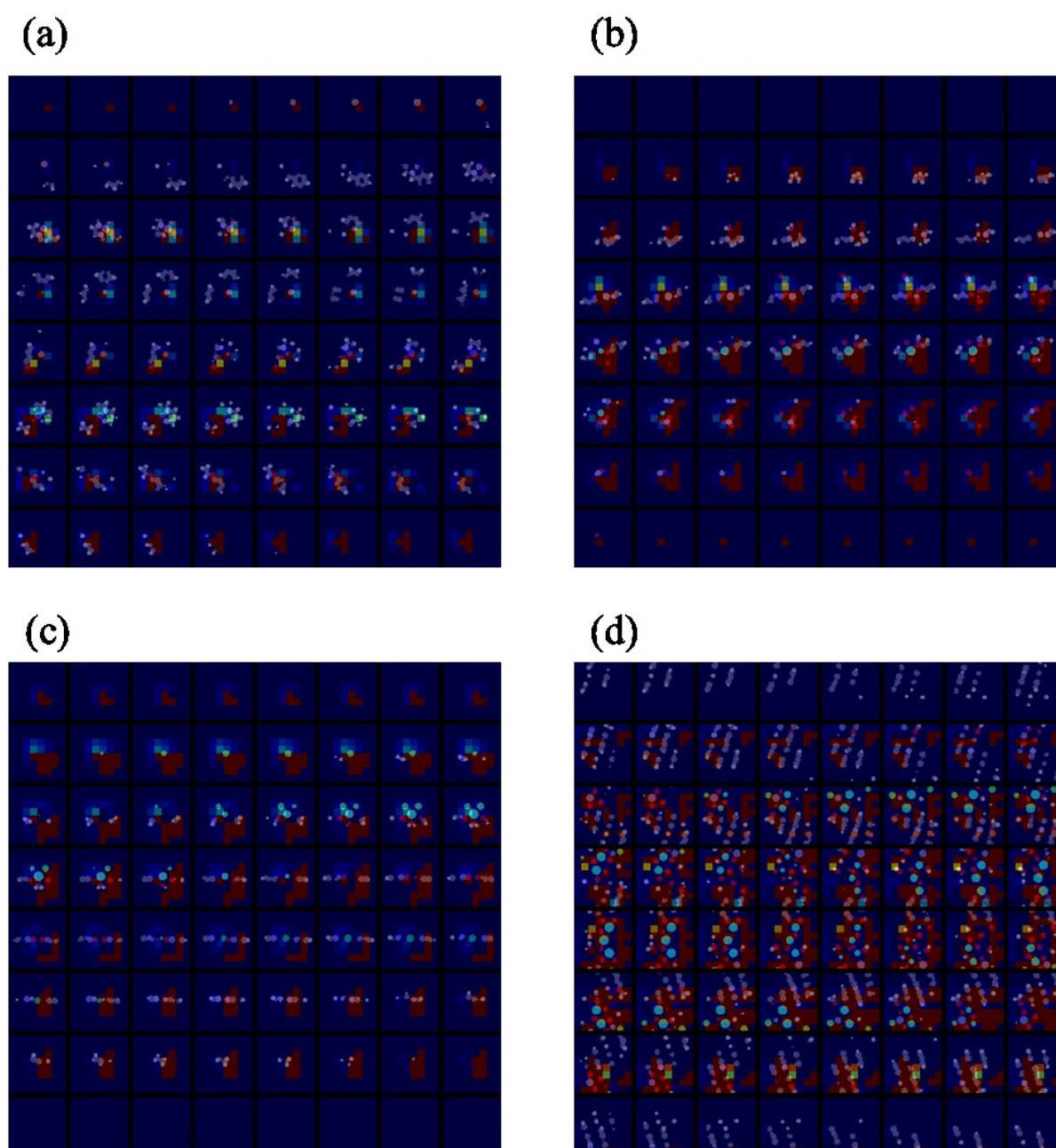


Figure S4 Each 3d-4f metal combinations in non-SMM molecules.



**Figure S5** Figure S5 Cross-entropy error (a) and correct answer rate (b) and AUC (c) as a function of the number of training epochs for the training dataset (blue trace) and validation dataset (orange trace).



**Figure S6** Visualization of CNN prediction results using Grad-Cam. a) Prediction: SMM, Result: SMM, b) Prediction: non-SMM, Result: non-SMM, c) Prediction: non-SMM, Result: SMM, d) Prediction: SMM, Result: non-SMM.