Electronic Supplementary Information (ESI)

## Predicting compositional changes of organic-inorganic hybrid

### materials with Augmented CycleGAN

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# Supplementary figures

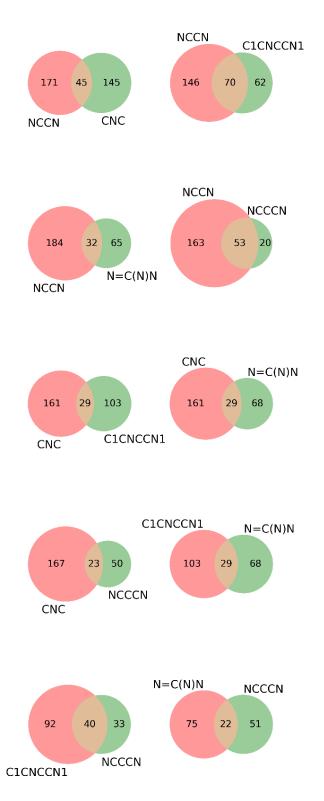


Figure S 1. Venn diagram of chemical systems found in structure groups.

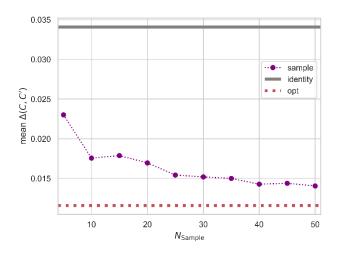


Figure S 2. Mean value of  $\Delta_{\text{sample}}$  as a function of  $N_{\text{sample}}$ .

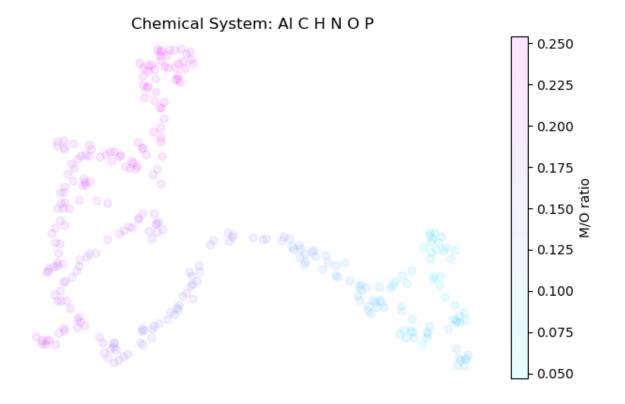


Figure S 3. Generated compositions of AI-C-H-N-O-P system colored by AI/O ratio. See Figure 9 in the main text for more details.

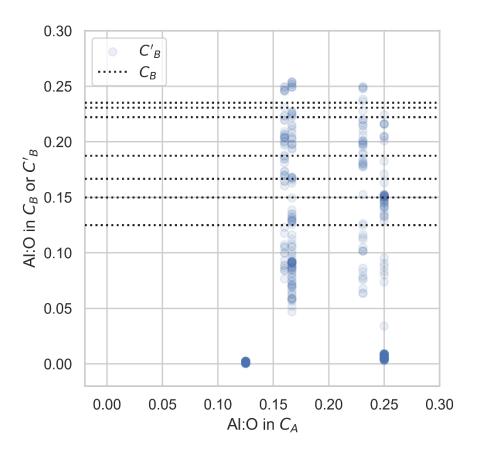


Figure S 4. Values of AI:O ratio of generated compositions of AI-C-H-N-O-P system.

#### CRediT

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QA: Methodology, Software, Data curation, Writing- Original draft, Visualization, Investigation.

JS: Supervision, Conceptualization, Writing - Review & Editing.

AN: Supervision, Conceptualization, Writing - Review & Editing.