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Supplementary Information for

Melting temperature prediction using a graph neural network model: from ancient minerals to new materials

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SI References

Other supplementary materials for this manuscript include the following:

Datasets S1 to S2

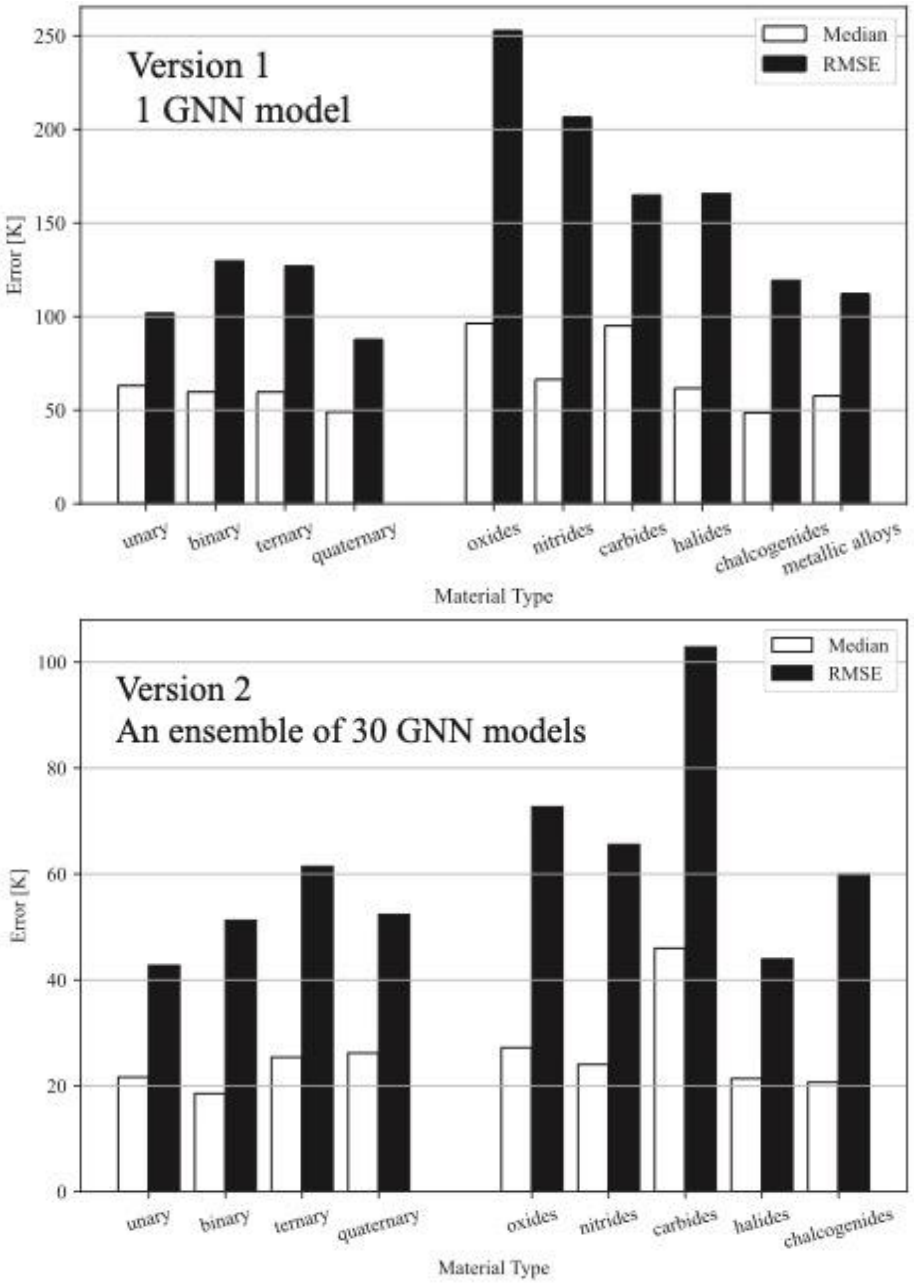

Fig. S1. Median error and root mean square error (RMSE) for materials of different types, evaluated over all data points. Stronger elemental interactions, as observed in oxides, nitrides, and carbides tend to incur relatively larger errors, since these contributions are diverse and more difficult to capture.

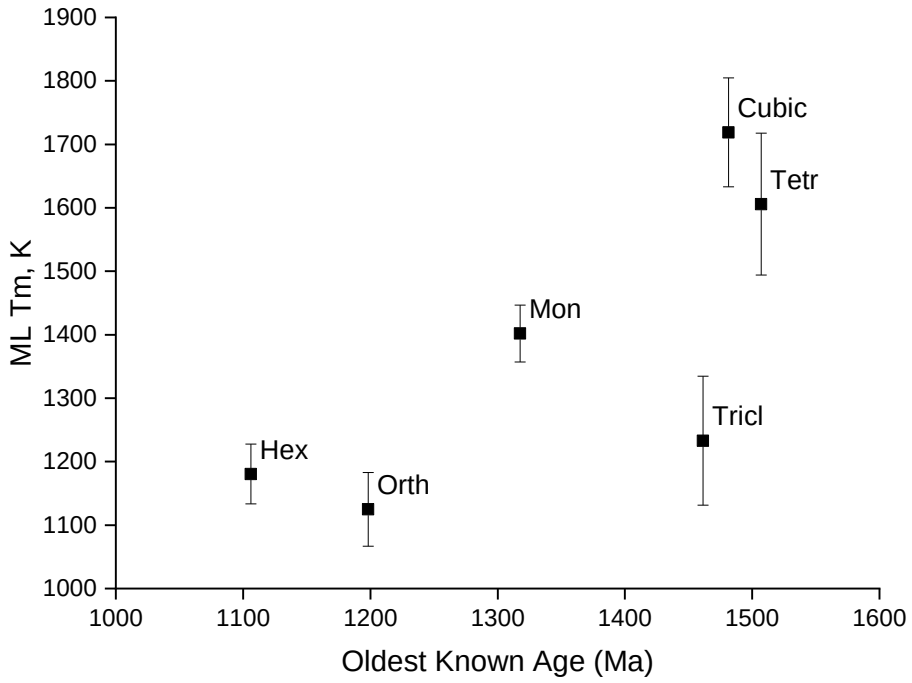

Fig. S2. Predicted melting temperature[1] vs. oldest known age for 401 rare earth containing minerals from RRUFF dataset (https://rruff.info/ima/)[2, 3], averaged by crystal system (cubic: 21; tetragonal: 23; orthorhombic: 80; hexagonal: 112, monoclinic: 138). Melting temperature model was built based on a dataset of 9375 compounds.

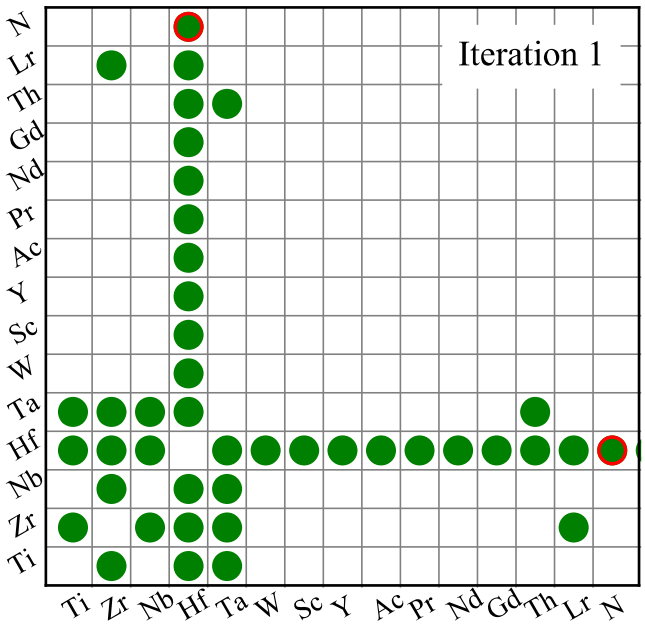

Fig. S3. Prediction of high melting temperatures in ternary systems, based on the GNN model[1] and MC simulated annealing. The top candidates are dominated by carbides and nitrides. The only exception is a carbonitride, the Hf-C-N system, which is exactly the material of the highest melting temperature predicted in 2015 based on DFT MD simulations.[4] The DFT melting temperatures of the Hf-C-N system were deliberately excluded from the database and ML model to test the method's predictive capability.

Legends for datasets

DATASET_S1_Minerals_ML_Tm_20220503.xlsx

Microsoft Excel spreadsheet with melting temperatures for 5793 mineral species calculated on May 8, 2022 using Melting Temperature Predictor Based on Machine Learning Graph Neural Networks (GNN).[1] The list of mineral species with compositions, crystal systems, and oldest known age was downloaded from RRUFF database (https://rruff.info/ima/)[2, 3] on 05/03/2022. The values of melting temperatures for compositions directly matched with the database used for training of GNN are selected in bold. Melting temperature model was built based on a dataset of 9375 compounds.

DATASET_S2_RE_minerals_ML_Tm_20220503.xlsx

Microsoft Excel spreadsheet with melting temperatures for 412 rare earth containing mineral species calculated on May 8, 2022 using Melting Temperature Predictor Based on Machine Learning Graph Neural Networks (GNN).[1] The list of mineral species with compositions, crystal systems, and oldest known age was downloaded from RRUFF database (https://rruff.info/ima/)[2, 3] on 05/03/2022. The structural complexity indexes received from S.V. Krivovichev (also partially available at https://info.deepcarbon.net//vivo/gemi_minerals Deep Carbon Observatory Data Portal).[5] The values of melting temperatures for compositions directly matched with the database used for training of GNN are selected in bold. Melting temperature model was built based on a dataset of 9375 compounds.

SI references

1. Hong, Q. J. Melting temperature predictor based on machine learning. https://faculty.engineering.asu.edu/hong/melting-temperature-predictor/ (accessed 6/02/2022).
2. Golden, J. J., Mineral Evolution Database: Data Model for Mineral Age Associations. . *M.S. Thesis, University of Arizona, Tucson AZ* **2019**.
3. Prabhu, A.; Eleish, A.; Zhong, H.; Fontaine, K.; Fox, P.; Morrison, S. M.; Hazen, R. M.; Huang, F.; Golden, J. J.; Downs, R. T.; Perry, S. N.; Hummer, D. R.; Ralph, J.; Runyon, S. E.; Krivovichev, S., Global earth mineral inventory: A data legacy. *Geosci Data J* **2021,** *8* (1), 74-89.
4. Hong, Q.-J.; van de Walle, A., Prediction of the material with highest known melting point from ab initio molecular dynamics calculations. *Physical Review B - Condensed Matter and Materials Physics* **2015,** *92* (2), 1-6.
5. Prabhu, A.; Morrison, S. M.; Eleish, A.; Zhong, H.; Huang, F.; Golden, J. J.; Perry, S. N.; Hummer, D. R.; Ralph, J.; Runyon, S. E.; Fontaine, K.; Krivovichev, S. V.; Downs, R. T.; Hazen, R. M.; Fox, P., Global Earth Mineral Inventory: A Deep Carbon Observatory Data Legacy. Version 1.0. DCO. (https://dx.deepcarbon.net/11121/6200-6954-6634-8243-CC). **2019**.