

HDNNP training data set for water

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This archive contains the full data sets required for training the high-dimensional neural network potential (HDNNP) ¹ for water presented in Ref. 2.

For each of the four models described in Ref. 2 there is a separate data set containing about 7000 configurations (see table below). Each set contains structures of seven ice phases (ice Ih, XI, IX, II, XIV, XV, VIII) and liquid water with 16, 32, 64 and 128 molecules.

Set	# of structures	Comment
input.data.BLYP	6996	BLYP functional
input.data.BLYP-D3	7183	BLYP functional with D3 corrections
input.data.RPBE	7258	RPBE functional
input.data.RPBE-D3	7241	RPBE functional with D3 corrections

Configurations are stored in the [RuNNer](#) configuration file format (see a description [here](#)) and can be used as an input file for training with [RuNNer](#) or [n2p2](#).

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| 1 | Behler, J.; Parrinello, M. Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces. <i>Phys. Rev. Lett.</i> 2007, 98 (14), 146401. https://doi.org/10.1103/PhysRevLett.98.146401 . |
| 2 | Morawietz, T.; Singraber, A.; Dellago, C.; Behler, J. How van Der Waals Interactions Determine the Unique Properties of Water. <i>Proc. Natl. Acad. Sci. U. S. A.</i> 2016, 113 (30), 8368–8373. https://doi.org/10.1073/pnas.1602375113 . |
| n2p2 | https://github.com/CompPhysVienna/n2p2 |
| RuNNer | http://www.uni-goettingen.de/de/560580.html |