Applications of Hamiltonian Dynamics for the representation of a loss function in search of new crystal structures

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Hamiltonian Dynamics are applied to obtain unbiased estimates of the Evidence Lower Bound and its gradients in search of new crystal structures of Si allotropes. We use the method of Hamiltonian Variational Auto Encoder (HVAE)[1] to generate a set of crystal replicas defined in a two-dimensional optimal continuous space using the information on the Radial Distribution Functions (RDF) of the known structures. Pearson correlation is computed to examine the similarity to database RDF and compared to the value acquired in searches using a standard VAE. It is found that the training proceeds more stably by means of HAVE (Figure 1). However, the correlation is increased only slightly.

Meanwhile, in attempts to accelerate the search of potentially stable materials we have tested the Module for ab initio structure evolution (MAISE) [2] for the generation of neural network models of interatomic potentials as an alternative tool to the Vienna Ab initio Simulation Package (VASP). In future, investigations based on graphical neural networks will be performed to utilize their flexible applications provided for the discovery of new materials.

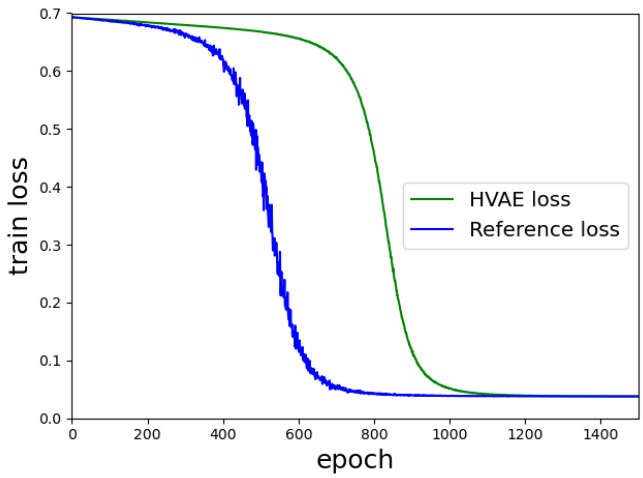

Figure 1 Training loss changes with the increasing number of epochs of a standard VAE (Reference loss) and HAVE (HAVE loss) models using 'SGD' optimizer for the generation of crystal replicas.

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References [1] Caterini et al., "Hamiltonian Variational Auto-Encoder," Proceedings of the 32nd International Conference on Neural Information Processing Systems, 8178–8188 (2018).

[2] Hazinazar et al., "MAISE: Construction of neural network interatomic models and evolutionary structure optimization, Computer Physics Communications, 259, 107679 (2021).