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Prediction of the Surface Energy from the Robust Extraction of Local Energy via Atomic Neural Network

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The prediction of the surface energy is crucial to the characterization of the morphology of various nanostructures and has been performed by density functional theory (DFT) calculations. Recently, the authors successfully developed the methodology to estimate the surface energy as a function of temperature and pressure by ab-initio thermodynamics [1, 2]. However, the calculation of the absolute value of the surface energy using this method is available only to the slab geometry whose top and bottom surfaces are identical with each other. It is noted that this condition is fulfilled only in very limited situations; at least one of the mirror, inversion, and rotoinversion symmetries must be present along the surface. If the surface of interest does not satisfy this condition, the surface energy of a slab cannot be calculated using the conventional method. In order to resolve this limited availability of surface energy calculations, the extraction of the correct local energy should be possible, which is not easy. In this study, the local energy within allowed error range was extracted from the DFT total energy with the help of atomic neural network (ANN). The ANN maps an atomic environment to the corresponding atomic energy. However, the obtained atomic energy is generally meaningless because the ANN training is the process to minimize the error in total energy not in atomic energy. Using GaAs polar surfaces as examples, we demonstrate that the robust extraction of the meaningful local energy and following surface energy is possible by the careful design of training datasets, descriptors, and network structure.

References

[1] I.W. Yeu, et al., Scientific Reports, 7 (2017), 10691.
[2] I.W. Yeu, et al., Scientific Reports, 9 (2019), 1127.