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일시 : 2022년 10월 13일 (목) 오후 5 : 00 장 소 : 이학관 331호

Machine-learned potentials: current status and perspectives

Recently, machine-learning (ML) approaches to developing interatomic potentials are attracting considerable attention because it is poised to overcome the major shortcoming inherent to the classical potential and density functional theory (DFT), i.e., difficulty in potential development and huge computational cost, respectively. In this presentation, based on in-house program SIMPLE-NN [1] for training and using neural network potentials (NNPs), we present our recent results on various material simulations: highly-efficient crystal structure prediction [2], accelerated computation of thermal conductivities [3], emission spectrum of quantum dots [4], electrocatalysts in fuel-cells, and simulation of semiconductor processing such as etching and atomic-layer deposition. We also discuss about a new avenue of material modeling that opens up by combining the machine learned potentials and various statistical approaches.

References

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2. S. Kang, W. Jeong et al, npj Computational Materials 8, 108 (2022).
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