Molecular dynamics simulation using machine-learning potential (기계학습 포텐셜을 이용한 분자동역학)

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Recently, machine-learning (ML) approaches to developing interatomic potentials are attracting considerable attention. In particular, the high-dimensional neural network potential (NNP) suggested by Behler and Parrinello is attracting wide interests. In this presentation, we first discuss on the fundamental aspect of ML potentials that enables the transferability of the potential. We show that the transferable atomic energy can be defined within the density functional theory, which means that the core of machine-learning potentials is to deduce a reference atomic-energy function from the given set of total energies. However, we also find that the neural network potential is vulnerable to 'ad hoc' mapping in which the total energy appears to be trained accurately while the atomic energy mapping is incorrect in spite of its capability.[1] The energy mapping in multi-component systems is also discussed. We also introduce our in-house code for training and executing NNP called SIMPLE-NN (SNU Interatomic Machine-learning PotentiaL packagE-version Neural Network) [2] and discuss its unique feature such as GDF weighting [3].