高次元ニューラルネットワークポテンシャルによる InN/AlN ヘテロ構造の研究

Study of InN/AlN Heterostructures with High-Dimensional Neural Network Potentials

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InN has the highest electron mobility among the group-III nitrides, which makes this material promising for various electronic device applications such as FETs. The use of AlN as a buffer layer is known to be effective to enhance the quality of InN layer. In order to reduce undesired defects and dislocations introduced during the growth process, theoretic understanding of structural and electronic properties of InN/AlN heterostructure is necessary.

Density functional theory (DFT) methods are powerful to obtain such an understanding. However, the conventional exchange-correlation functionals often fail to predict the semiconducting nature of InN. We use the pseudo-self-interaction correction (pSIC) [1] to eliminate the spurious self-interaction of localized electrons, which gives an accurate band gap for InN. Besides, the heavy computational load of DFT calculations makes it challenging to fully examine the defect or dislocation properties in large supercells. Therefore, we adopt the high-dimensional neural network potential (HDNNP) [2], which could reduce computational costs by several orders of magnitude yet maintain comparable accuracy with DFT calculations. Note that the application of HDNNP to multiple charge states has not been considered in previous studies. Thus, we introduce a way to construct HDNNP for group-III nitrides with multiple charged defects.

In this study, the pSIC method was confirmed to describe the electronic band structures of InN and AlN accurately. Then we developed the HDNNP applicable to InN/AlN systems in neutral charge state, and we revealed the finite size effects in supercells containing single neutral, +1 or +3 N vacancy. More importantly, the HDNNP for InN/AlN systems in multiple charge states was constructed successfully.

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