PURDUE INNOVATES | Office of Technology Commercialization

DFTB Parameterization Method to Faithfully Reproduce Various Observables

An electronic model reliably predicts the tunable piezoelectric activity of stacked two-dimensional materials for use in nanoelectronics and nanoelectromechanical systems.

Researchers at Purdue University have developed a density-functional tight-binding (DFTB) method for predicting piezoelectric coefficients of fully relaxed, twisted 2D heterobilayer materials. Piezoelectric materials have applications in nanoelectromechanical systems and nanoscale electronics. 2D monolayers have piezoelectric activity. Stacking monolayers provides higher piezoelectricity than the sum of the piezoelectricity of the monolayers. The twist angle between the layers can be tuned. The Purdue researchers created an electronic model to predict the piezoelectric coefficient of corrugated and twisted 2D heterobilayer systems. The model predicts the relationship between piezoelectric coefficient and twist angle.

Technology Validation: In an untwisted hBN/hBP heterobilayer, the model reproduces all relevant piezoelectric bands obtained from DFT.

Advantages

- Model gives reliable convergence in contrast to small-supercell limited DFT

Applications

- Prediction of piezoelectric activity in heterobilayers

TRL: 2

Intellectual Property:

Provisional-Patent, 2022-07-13, United States | Utility Patent, 2023-07-13, United States | Copyright, N/A, United States

Keywords: Density-functional tight-binding, DFTB, piezoelectric coefficients, twisted 2D heterobilayer materials, nanoelectromechanical systems, nanoscale electronics, 2D monolayers, piezoelectric activity, twist angle,

Technology ID
2022-KUBI-69916

Category
Semiconductors/Devices & Components
Materials Science & Nanotechnology/Nanomaterials & Nanostructures
Materials Science & Nanotechnology/Advanced Functional Materials

Authors
Han-Wei Hsiao
Tillmann C Kubis

Further information
Dipak Narula
dnarula@prf.org

View online

electronic model, Heterobilayer, Materials and Manufacturing, Monolayer, Piezoelectric, Twist angle