SPECIAL TOPIC — Smart design of materials and design of smart materials

Machine learning of the Γ-point gap and flat bands of twisted bilayer graphene at arbitrary angles

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The novel electronic properties of bilayer graphene can be fine-tuned via twisting, which may induce flat bands around the Fermi level with nontrivial topology. In general, the band structure of such twisted bilayer graphene (TBG) can be theoretically obtained by using first-principles calculations, tight-binding method, or continuum model, which are either computationally demanding or parameters dependent. In this work, by using the sure independence screening sparsifying operator method, we propose a physically interpretable three-dimensional (3D) descriptor which can be utilized to readily obtain the Γ-point gap of TBG at arbitrary twist angles and different interlayer spacings. The strong predictive power of the descriptor is demonstrated by a high Pearson coefficient of 99% for both the training and testing data. To go further, we adopt the neural network algorithm to accurately probe the flat bands of TBG at various twist angles, which can accelerate the study of strong correlation physics associated with such a fundamental characteristic, especially for those systems with a larger number of atoms in the unit cell.

Keywords: twisted bilayer graphene, band gap, flat bands, machine learning

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1. Introduction

Graphene has attracted a tremendous amount of interest due to its unique structure and outstanding physical properties, which can be further tuned via forming twisted bilayer graphene (TBG).[1,2] Recently, TBG has become a new platform for probing the band topology, the electronic correlations, the van Hove singularities, the quantum Hall effect, *etc*.[3–9] In particular, the electronic bands of TBG near the Fermi level become extremely flat around the first magic angle of 1.08°,[10–16] where unconventional superconducting[17] and charge-ordered states[18] have been observed. In general, TBG exhibits four flat bands near the Fermi level which are separated from others by energy gap. To quantify such "flatness" of band structure, reliable evaluation of the gap between non-flat bands at the Γ-point (Brillouin zone center) is of great importance.[19–23] For convenience, we name it as "Γ-point band gap" in the following discussion. Theoretically, the electronic structure of TBG can be calculated by using the density functional theory,[24,25] the full tight-binding method,[26–28] or the simplified continuum model.[29–31] While reliable results could be obtained for systems with specific twist angles, these approaches are either computationally prohibitive or parameters dependent. It is thus quite necessary to find alternative solutions to such a fundamental problem so that the Γ-point band gap of TBG at arbitrary angles can be accurately and readily determined.

As known, machine learning (ML) is a data-driven approach that has been widely used in many important fields of physics, chemistry, and material science. In particular, several ML models[32–40] have been recently proposed to effectively evaluate the energy band gap in a high-throughput way. For instance, Pilania *et al.* utilized a cross-validated kernel ridge regression (KRR) model to reliably predict the band gaps of double perovskites.[32] Zhuo *et al*. proposed a support vector regression (SVR) model for band gaps of inorganic solids, where the 136 input features were constructed based on the elemental properties of the constituent atoms.[33] Huang *et al.* developed an SVR model to accurately obtain the band gaps of nitrides in a large design set, achieving a root mean square error (RMSE) as small as 0.005 eV.[35] For the two-dimensional systems, Ma *et al*. combined active learning with high-throughput *ab-initio* calculations to screen out hexagonal binary compounds with proper photovoltaic band gaps.[37] To accelerate the discovery of promising photocatalytic and photovoltaic candidates, Sa *et al*. used the crystal graph convolutional neural network (CGCNN) model to reliably predict the gaps of 1035 Janus III–VI vdW heterostructures.[38] In the case of TBG, however, the ML approaches for the accurate prediction of the energy

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gap at the Γ-point and especially the flat bands are less known so far.

In this work, we use the data-driven Sure Independence Screening and Sparsifying Operator (SISSO) method[41,42] to quickly and accurately predict the Γ-point gap of TBGs at various twist angles. Moreover, we adopt the neural network (NN) algorithm[43] to probe the corresponding energy eigenvalues at negligible computational cost. Collectively, our approaches could accelerate discovery of many potential TBGs with distinguished flat bands around the Fermi level.

2. Computational method

We employ the SISSO approach to derive an efficient descriptor for predicting the Γ-point gap of TBGs. Here, the input features include several structural parameters such as the twist angle (θ), the interlayer spacing (d), and the characteristic index (M,N) of TBG. All of them are combined by iteratively using the chosen algebraic operators $H = \{I,+,-,\times,/,\exp,\log,|-|,\sqrt{},^{-1},^{2},^{3}\}$, which could lead to a very huge feature space. The sure independence screening (SIS) is then adopted to select the subspace that contains descriptors highly correlated with the target property (band gap). After the dimensionality reduction, we use the sparsifying operator (SO) to obtain the optimal three-dimensional (3D) descriptor. Compared with many other ML algorithms, the SISSO-derived descriptors are explicit and analytic functions of several key inputs, which is very beneficial for understanding the associated physical mechanisms.

In addition to the SISSO method, we employ the NN algorithm to develop a high-throughput model for predicting the energy eigenvalues of TBGs at various twist angles. In general, the architecture of NN includes the input unit, the hidden layers, and the quantitative labels of target values as output unit. In the present work, the rectified linear units (Relu) and the mean square error (MSE) are chosen as the activation function and loss function, respectively. During the NN training process, we have carefully checked the hyperparameters such as the batch size, the number of hidden layers and the corresponding neurons. We find that using 3 hidden layers (each with 256 neurons) and a batch size of 128 could ensure high prediction accuracy of our NN model.

3. Results and discussion

As known, TBG is formed by two layers of graphene with a specific twist angle θ, coupled via van der Waals interaction. Figure 1(a) shows the crystal structure of TBG, where the commensurate lattice vectors of the Moiré unit cell are defined in terms of two positive integers (M,N) and the primitive lattice vectors of graphene ($\boldsymbol{a}_1$ and $\boldsymbol{a}_2$). That is: $\boldsymbol{R}_1 = N\boldsymbol{a}_1 + M\boldsymbol{a}_2$ and $\boldsymbol{R}_2 = -M\boldsymbol{a}_1 + (N+M)\boldsymbol{a}_2$. Consequently, the twist angle of a given TBG can be written as $\cos\theta = \frac{N^2+4NM+M^2}{2(N^2+NM+M^2)}$. As mentioned above, we adopt the SISSO approach to give an accurate prediction of the band gap ($E_{\rm pre}$) of TBG at various twist angles. As mentioned above, the gap is generally assumed as the energy difference between the non-flat bands at the Γ-point. To construct a reliable training set, we have collected 50 Γ-point gap values of TBG at different twist angles, as shown in Fig. 1(b). Note that they were obtained from first-principles calculations, the tight-binding method, the continuum model, *etc.*,[10–16,19–29,44–66] depending on the number of atoms in the Moiré unit cell of TBG. Among the 50 entries, we see from Fig. 1(b) that most TBGs exhibiting twist angles in a narrow range of 0°–3°. In principle, such a non-uniform distribution of training data with small size is actually not beneficial for ML. Fortunately, the problem can be effectively addressed by adopting the semi-supervised learning (for example, self-training), as discussed in the following.

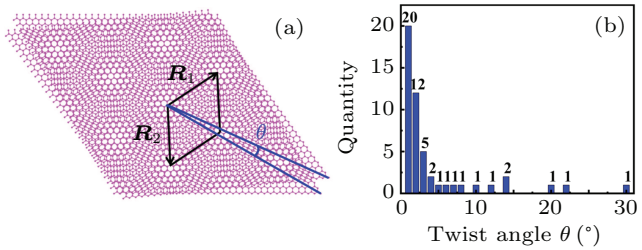


Fig. 1. (a) Illustration of the crystal structure of TBG, where θ is the twist angle and $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ are the commensurate lattice vectors of the Moiré unit cell. (b) The distributions of initial 50 TBGs according to their twist angles.

For any ML method, the selection of input features plays a crucial role in determining an efficient data-driven model. Our extensive checks in a huge feature space indicate that, using only the twist angle θ, the interlayer spacing d, and the characteristic index (M,N) of TBG is enough to pinpoint an optimal descriptor for the accurate prediction of the Γ-point gap. As the gap values in the training data span over several orders of magnitude, we choose the log-scale for the convenience of training. By training the original 50 Γ-point gaps ($\log E_{\rm real}$), our SISSO approach could derive an initial descriptor, which is subsequently used to predict the gaps of few unlabeled samples (for example, 5 new TBGs). Such a self-training process is iteratively executed until the relative RMSE of the descriptor reaches an acceptable tolerance level. Specifically, by gradually increasing the size of training data from 50 to 125, a robust and optimized SISSO descriptor can be determined in a 3D form

$$\log E_{\rm pre} = -12.27 \times D_1 - 8.6 \times 10^{-3} \times D_2 + 0.01 \times D_3 + 5.4, \quad (1)$$

where D_1, D_2, and D_3 are defined as

$$D_1 = \theta^{-1/4} \times d^{-1}, \quad (2)$$

$$D_2 = \exp(N^{-1}) \times \frac{M}{N} \times \exp(d), \quad (3)$$

$$D_3 = \left|\exp(d) - \exp\left(\theta^{-1}\right)\right|. \quad (4)$$

Figure 2(a) shows the quantitative comparison of the 125 gaps of TBG in the training set ($\log E_{\text{real}}$) and those predicted by the 3D descriptor ($\log E_{\text{pre}}$). We see that all the data points are evenly distributed around the dashed line indicating the equality, which suggests higher prediction accuracy of our SISSO descriptor. Indeed, the Pearson correlation coefficient between $\log E_{\text{real}}$ and $\log E_{\text{pre}}$ can be reached to 99%. Besides, we have performed the leave-one-out cross-validation, and the best descriptor given in Eq. (1) can be always identified in 92% of 125 iterations. All these findings suggest the strong predictive power of the SISSO-derived 3D descriptor.

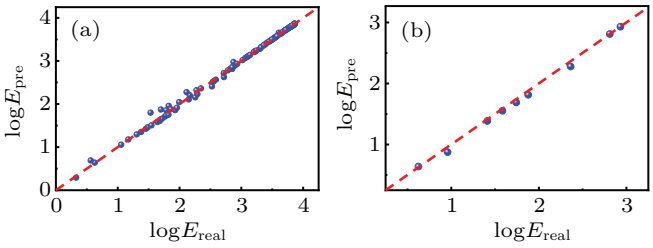


Fig. 2. The intuitive linear correlation between the SISSO-predicted log-scaled band gaps of TBG and those from previous calculations for (a) 125 training data, and (b) 9 new TBGs. The red dashed line represents the equality.

Unlike many ML models which appear as black box, the SISSO-derived descriptor in the present work is physically interpretable for predicting the Γ-point gap of TBG. With a detailed analysis of each term in Eq. (1), we find $-12.27 \times D_1$ and $0.01 \times D_3$ play major roles in determining the $\log E_{\text{pre}}$. At fixed interlayer spacing d, we see from Eq. (2) that D_1 decreases with increasing twist angle θ, and in turn leads to a large $\log E_{\text{pre}}$. Besides, equation (4) can be rewritten as $D_3 = \exp(d) - \exp\left(\theta^{-1}\right)$ at large θ, which means that D_3 increases with θ, and also gives rise to a large $\log E_{\text{pre}}$. If the twist angle θ is small, we have $D_3 = \exp\left(\theta^{-1}\right) - \exp(d)$, which exhibits competing behavior with D_1 so that the variation of $\log E_{\text{pre}}$ with θ is non-monotonic. All these observations are consistent with previous tight-binding results.[11,44] On the other hand, if the twist angle θ is fixed, we can find from Eq. (2) that D_1 increases with decreasing interlayer spacing d, leading to a small $\log E_{\text{pre}}$.[19] Meanwhile, it is obvious that at large θ, reducing interlayer spacing d leads to decreased D_3 and thus a small $\log E_{\text{pre}}$. Such behavior becomes inversed at small θ, which is however corrected by the major contribution from the first term of Eq. (1) ($-12.27 \times D_1$). As a consequence, a lower $\log E_{\text{pre}}$ value can be expected at decreased d, no matter the θ is large or small. The physical reason is that the compression of interlayer spacing enhances the electronic coupling between the layers of TBG, and a smaller band gap can be thus expected.[19,21,67]

Beyond the training data, the SISSO-derived descriptor is employed to predict the Γ-point gaps of 9 TBGs ($\log E_{\text{pre}}$), as shown in Fig. 2(b). For comparison, the results obtained from previous theoretical calculations or experimental measurements[11,45,57,60,64–69] are also given ($\log E_{\text{real}}$). It can be found that $\log E_{\text{pre}}$ almost coincide with $\log E_{\text{pre}}$ and the calculated Pearson correlation coefficient is as high as 99%. For instance, the Γ-point gap of TBG with $\theta = 0.37^\circ$ is 4.2 meV according to the photocurrent measurement,[60] which is very close to our SISSO-predicted value of 4.3 meV. On the theoretical side, it was previously found that the gaps of TBG at $\theta = 0.6^\circ$ and 3.0° are respectively 26.1 meV and 644.7 meV,[64,65] which show good agreement with our SISSO predictions of 24.3 meV and 647.1 meV. All these results further confirm the good reliability of the data-driven descriptor in predicting the Γ-point gap of TBG. As the D_1, D_2, and D_3 terms in Eq. (1) contain only four structural parameters of TBG (θ, d, M, N), our 3D descriptor could give high-throughput prediction of gaps for numerous TBGs at arbitrary twist angles and interlayer spacings. For example, we can create 2716 unique TBGs by varying the θ from 0° to 60° (with an interval of 0.2°) and d from 2.5 Å to 3.8 Å (with an interval of 0.1 Å). Among them, nearly half (1308) are found to exhibit small Γ-point gap (0 eV–1 eV), which suggests that they may have characteristic of flat bands.[11,21] Figure 3 plots the distribution of these 1308 TBGs according to their twist angles and interlayer spacings. It is interesting to find that such narrow range of gap can only be realized at $\theta < 15.2^\circ$. In another word, for TBGs with $60^\circ > \theta > 15.2^\circ$, the corresponding gaps are larger than 1 eV and thus not shown. Besides, we see that the corresponding range of θ becomes small with increasing d. For example, at $d = 2.5$ Å, we observe a wide range of 0.2°–15.2° , which is significantly reduced to 0.2°–2.65° at large d of 3.8 Å. Collectively speaking, our results shed some light on designing TBGs that could exhibit flat bands at various combinations of twist angle and interlayer spacing.

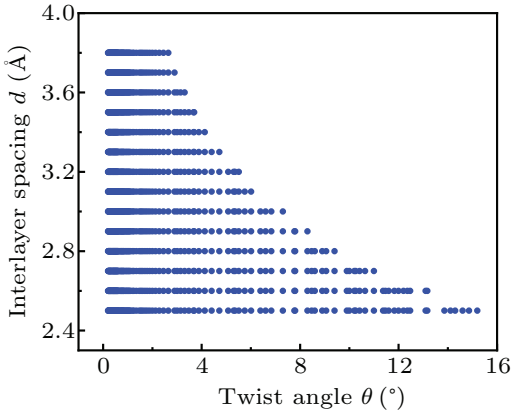


Fig. 3. The distribution of 1308 TBGs with predicted band gaps in the range of 0 eV–1 eV, plotted as a function of their twist angles and interlayer spacings.

Although our SISSO-derived descriptor can be utilized to accurately predict the Γ-point gap of TBG, it alone is not sufficient to identify the existence of flat bands. To give

a direct prediction of energy bands around the Fermi level, we construct a dataset of 31 TBGs that exhibit 4 obvious flat bands along the K–Γ–M–K' path in the first Brillouin zone.[11–13,19,20,26,28,46,56,64,69] For each band, 150 $\boldsymbol{k}$ points are considered so that a total of 18600 energy eigenvalues can be obtained. As an alternative, we adopt the NN algorithm since it has obvious advantage in dealing with a large amount of data. Here, the input features are the same as before, and by default, the indices of band and $\boldsymbol{k}$ points are also included. We find that best performance of NN model can be obtained when 90% of the dataset is randomly selected for training and the remaining 10% for testing. Indeed, both of them exhibit a very high Pearson correlation coefficient of 99.8% between the predicted energy eigenvalues and those calculated in previous works.[11–13,19,20,26,28,46,56,64,69] Besides, the RMSE of the training and testing set are found to be as small as 12.3 meV and 12.0 meV, respectively. To go further, we show in Fig. 4 the NN-predicted flat bands of two TBGs with twist angles of 1.35° and 2.65°. For both cases, it is found that our results almost coincide with those calculated by tight-binding method.[12,26] All these results demonstrate good accuracy of our NN model, which can be thus utilized to readily screen candidates with desired flat bands from a large pool of TBGs at arbitrary twist angles and interlayer spacings.

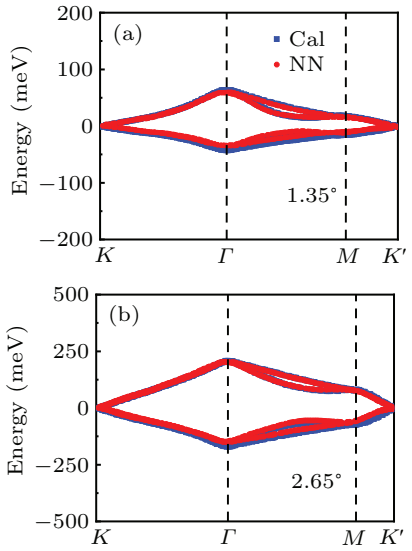


Fig. 4. The flat bands of TBG at two typical twist angles: (a) 1.35° and (b) 2.65°. Results predicted by the NN model and those from previous calculations are both shown for comparison.

4. Summary

In summary, by adopting the SISSO and NN algorithms, we propose high-throughput models to accurately predict the Γ-point gap and flat bands of TBG at arbitrary twist angles and interlayer spacings. Such a task could be computationally prohibitive by density functional calculations, or insufficient accurate by parameters-dependent tight-binding method. In principle, the strategies established here can be generalized to other various 2D twisted materials, provided enough data is available. It is expected that our work could provide a new insight to explore twisted bilayers with flat bands, which is of crucial importance in the study of correlated insulating and superconducting states.

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