Simulation of graphene based macromaterials: the influence of flake properties and atomic intercalation

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The excellent properties of graphene can be utilized in macroscopic conductor materials if the individual flakes are decoupled from each other, for example by misalignment of the lattices or by intercalation.

We show the results of a network model [1] to assess the properties of the macromaterial (Fig. 1 left) as a function of relevant parameters such flake size, packing density, the graphene flake conductivity, and the interlayer conductance. The model allows us to evaluate the anisotropy of the current flow in the in-plane and the out-of-plane directions of the graphene-based macromaterial [2].

Intercalation of the graphene-based macromaterial with additional atoms or molecules can also be used to enhance the material properties [3]. We show density functional theory calculations of graphite intercalated with AlF_3 and discuss the decoupling as well as the modulation of the electronic properties of the graphene flakes. Fig. 1 right shows the band structure before and after the intercalation with AlF_3.

References

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Figures

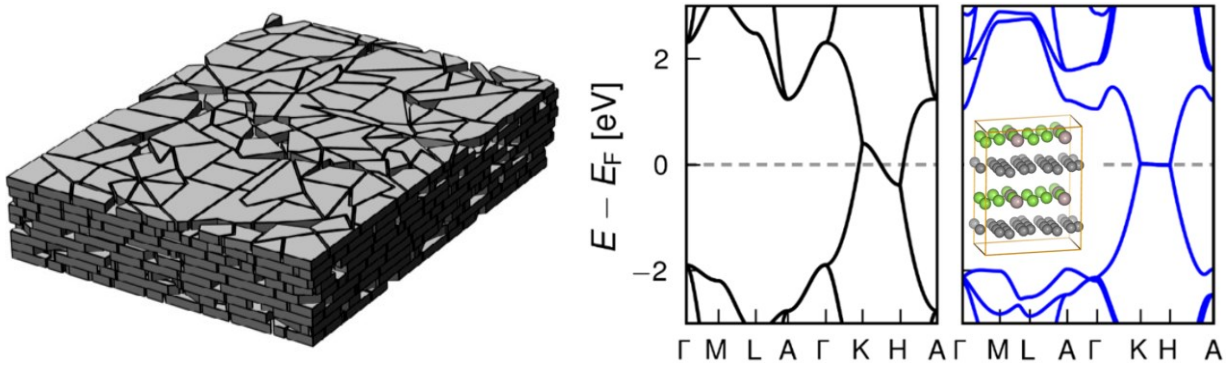

Figure 1: Left: Model system of a graphene based macromaterial. Right: Band structure of AA-stacked graphite without and with AlF_3. A 2×2×2 repetition of the model system is given in the inset.