Molecular dynamics with machine-learning potentials for describing defect dynamics in graphene and diamond

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Classical molecular dynamics (MD) is one of the few computational methods capable of modeling carbon materials with atomic resolution on nanosecond time scales. However, the development of a universal interatomic potential for carbon has long remained a challenging task due to the large variety of its allotropic forms. Potential models available only a few years ago did not provide sufficient accuracy [1]. Fortunately, recent advances in machine-learning–based interatomic potentials have significantly improved the accuracy of simulations of amorphous carbon [2], diamond [3], and more exotic carbon phases [4].

In the present work, using one of these potentials, we investigated the relationship between surface waves in graphene (the so-called intrinsic graphene ripples [5]) and the diffusion process of a single vacancy during long MD simulations (up to 0.5 ns) (Fig. 1). It is shown that neglecting the collective motion of the graphene sheet leads to an overestimation of the migration energy barrier by tens of percent. The obtained results may explain the significant spread in the literature values of this barrier, which, according to various sources, ranges from 0.5 to 1.4 eV. The presentation will also discuss the general capabilities of modern machine-learned interatomic potentials for predicting the properties of carbon.

References

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Figures

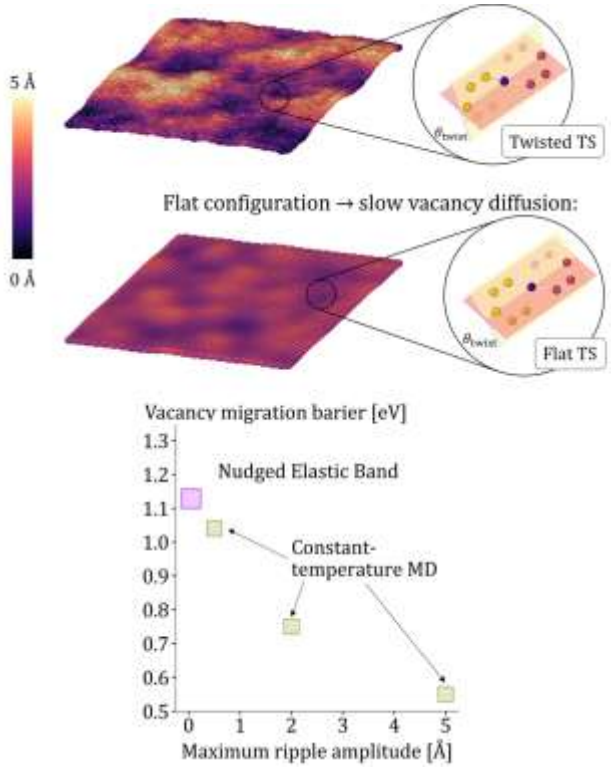

Figure 1. Influence of out-of-plane graphene motion (intrinsic rippling) on the monovacancy diffusion barrier in graphene.