Machine-learning Based Non-Adiabatic Molecular Dynamics for Nano-porous Graphene

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Nano-porous graphene (NPG) offers great potential for a variety of applications from electronics to photocatalysis. Its band gap can be tuned over a wide range of values, just by changing structural parameters [1]. Often, only ground-state properties have been studied for NPG. However, in order to optimize NPG for photo-physical and photo-chemical applications, their excited-state properties need to be studied. One method to study dynamic excited-state properties is non-adiabatic molecular dynamics (NAMD). Unfortunately, conventional NAMD employing *ab-inito* methods to describe ground- and excited-state potential energy surfaces is computationally expensive, particularly for periodic systems. Employing machine-learning methods can significantly reduce the computational cost of NAMD without compromising accuracy [2].

In this work, we trained machine-learning interatomic potentials for the ground state and the five lowest excited states for a specific NPG. We used these potentials to run NAMD simulations for the NPG, describing the transitions between states using Landau-Zener surface hopping [3]. Our findings show that the number of excited states included in the NAMD simulations affects the relaxation to the ground state. Furthermore, our NAMD simulations reveal the limitations of the chosen approach to NAMD simulations. Together with the advantages of the approach employed in this work, the limitations, possible solutions, and potential further developments will be discussed in this contribution.

References:

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