

Machine learning is a rapidly growing area that has recently gained ground in electronic structure simulations. Conventionally, density functional theory is the most prominent method of electronic structure method but requires one of the highest demands on academic high performance computing systems worldwide. Accelerating these with machine learning reduces the resources needed and allows for simulations of complex systems. Physics-informed neural network can be employed to determine the electronic structure and calculate the adhesion ability and identify types of surface interaction of polymers angelica lactone (ALP) and polymethyl methacrylate (PMMA). ALP is a green (biodegradable) polymer that is capable of polymer assisted transfer of graphene, which is important for graphene device fabrication. The task of the simulation is to see if the ALP binds to graphene more strongly in the presence of PMMA, which could be due to an increase of the Van der Waals interactions of graphene with angelica lactone by increasing the electrostatic forces between the polymers. Success will be measured by comparing the interaction energy of this method with DFT. Another measure of success will be comparing this method's CPU clock time with DFT.