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Molecular Dynamics Study of Amorphous Carbon

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EXTENDED ABSTRACT: With the rapid development of computer science, molecular dynamics has become an important means to study the structure, physical and chemical properties of matter at the atomic scale. Since amorphous silicon has multiple hybridization formats, it can form various types of structures and can exhibit a range of properties. Classical molecular dynamics has the characteristics of low computational cost and large time and space scales that can be simulated, so it has become a common method for studying amorphous carbon. Some interatomic potential functions for carbon have been proposed, such as Tersoff[1], EDIP[2] and so on. However, since the interatomic potential energy functions used in classical molecular dynamics are generally semi-empirical, the accuracy of the calculation results is often not high. Ab initio molecular dynamics(AIMD) can overcome this shortcoming, because the potential function in AIMD is obtained by the method of quantum mechanics. However, due to the complex iterative steps of AIMD, the computational cost is high, and it is difficult to simulate large time and space scales. The method of machine learning can combine the advantages of the two, which is also a current research trend. We used MD and AIMD to build models of amorphous carbon at different densities, and calculated their RDF and hybridization fractions. The model was built using the liquid quenching method. Calculations of the hybridization fraction show that it is a function of density, Figure 1 show the result of hybridization fraction.And as for the RDF calculations, there is always a peak at about 1.5 angstroms.

Keywords： amorphous carbon; molecular dynamics; machine learning

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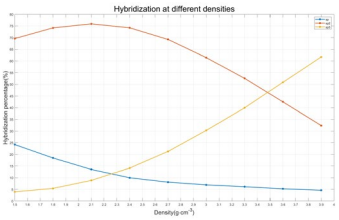

Figure 1. hybridization fraction of different densities of amorphous carbon.

BIOGRAPHY

Wang Rui has completed his bachelor's degree at the age of 22 years from Hefei University of Technology. Currently a master student at University of Science and Technology of China, under the tutelage of Professor Ding Zejun.