ELECTRONIC STRUCTURE SIMULATIONS OF HAEMOGLOBIN AND HAEMOZOIN

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ABSTRACT

One of the most devastating infectious diseases in the world, malaria poses a serious public health problem with at least 300 million people infected with the malaria parasite and more than one million dying globally each year. The Plasmodium falciparum infects the haemoglobin part of the blood releasing haem groups which are then agregated into a crystalline material called haemozoin.

In this work we present electronic structure calculations of the haemoglobin and the haemozoin molecules. Changes in the magnetic and structural properties of the iron in this environment are also reported.

Finally an attempt to identify and understand the nature of the electronic structure changes in the haemoglobin to haemozoin conversion using relativistic methods will be discussed.