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Structure and Formation of Synthetic Hemozoin: Insights from First Principles Calculations NOA MAROM, University of Texas at Austin, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut, Berlin, SERGEY KAPISHNIKOV, LEEOR KRONIK, LESLIE LEISEROWITZ, Weizmann Institute of Science, Israel — Malaria has reemerged due to parasite resistance to synthetic drugs that act by inhibiting crystallization of the malaria pigment, hemozoin (HZ). Understanding the process of HZ nucleation is therefore vital. The crystal structure of synthetic HZ, β-hematin (βH), has recently been determined via x-ray diffraction. We employ van der Waals (vdW) corrected density functional theory to study the βH crystal and its repeat unit, a heme dimer. We find that vdW interactions play a major role in the binding of the heme dimer and the βH crystal. Accounting for the βH periodicity is a must for obtaining the correct geometry of the heme dimer, due to vdW interactions with adjacent dimers. The different isomers of the heme dimer are close in energy, consistent with the observed pseudo-polymorphism. We use these findings to comment on βH crystallization mechanisms.

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