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First principles simulations of nano-peptides on copper surfaces.[1]
DUY LE, TALAT S. RAHMAN, University of Central FLorida — Protein folding is the process in which a protein structure finds its stable conformation or functional shape. It is considered as a robust way for self-assembling proteins into conformations with desired functionalities. In this work, to obtain a microscopic understanding of the protein folding phenomenon, as influenced by a metallic environment, we perform density functional theory based simulations of the folding of a 9-amino-acid nano-peptide on various copper surfaces. We show that the considered nano-peptides fold into stable monomers or dimers with different conformations depending on the crystallographic orientation of the surface. Comparison of our simulated Scanning Tunneling Microscopy (STM) image with available experimental results [1] provides insights into the microscopic forces responsible for dimerization on Cu(100). [1] S. Rauschenbach et al., to be published

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