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Publication date:
2017

Document Version
Publisher's PDF, also known as Version of record

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Citation (APA):

Zhang, L., Kepp, K. P., Ulstrup, J., & Zhang, J. (2017). *Ligations of Gold Atoms with Iron Porphyrin*. Abstract from Forth EuCheMS Inorganic Chemistry Conference (EICC-4), Copenhagen, Denmark.

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Ligations of Gold Atoms with Iron Porphyrin

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Gold is an exotic material with *d*-electrons deciding electronic mappings and configurations of adsorbed molecules.¹ The specific interaction of Au atoms and S-, N-capped molecules make gold nanoparticles widely applied in the medicine transport and immunoassay.^{2,3} Density functional theory demonstrates that the electronic structure of Au adatoms is d^9s^1 but not $d^{10}s^0$ in the forms of Au-thiolates.¹ The surrounding Au surface atoms are passivated leading to both Au-Au and S-S interactions. A wide range of surface phenomena of nanoparticle size-control and break-junctions in surface physics and chemistry including electrochemistry and electrochemical scanning tunneling microscopy (*in situ* STM) are explained with this theory.⁴

Iron porphyrin is a well-known active redox center of cytochrome *c* and hemoglobin/myoglobin assisting membrane-crossing electron transfer or blood oxygen transport.⁵ The electronic states and configurations of iron porphyrin affect the electrochemical properties of the metalloproteins, where the artificial constructed proteins are designed by the mutations of amino residues or the structural optimizations of iron porphyrins.⁶

Iron porphyrin adsorption on graphite and graphene surfaces by π - π electron stacking has been widely studied and the catalytic activity found to be enhanced warranting the notion of enzyme mimics.⁷ Weak physisorption was, however, recently observed by *in situ* STM,⁸ but the electronic properties of iron porphyrin adsorbed on gold has not been addressed before. This issue is, however, critical. We report here a study of iron porphyrin on the three low-index Au-surfaces using a combination of electrochemistry and density functional theory (Figure 1).

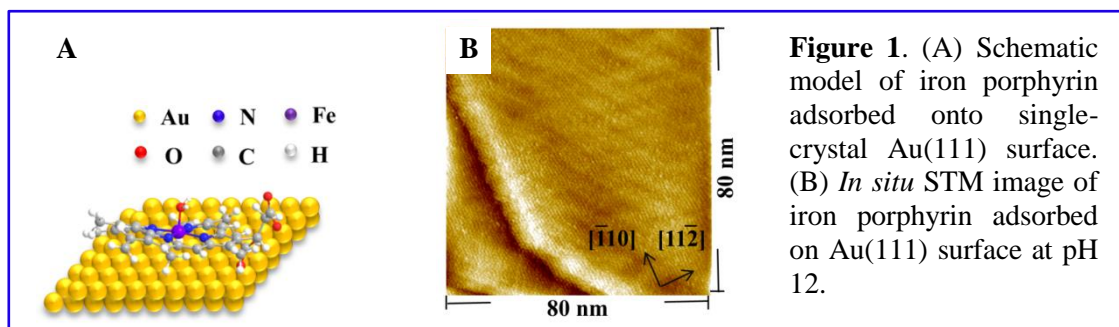


Figure 1. (A) Schematic model of iron porphyrin adsorbed onto single-crystal Au(111) surface. (B) *In situ* STM image of iron porphyrin adsorbed on Au(111) surface at pH 12.

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