

Heterogeneous Adsorption and Local Ordering of Formic Acid on a Magnetite Surface

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Magnetite (Fe_3O_4) is an important and diverse transition metal oxide with applications as a catalyst in various industrial processes such as the water-gas shift reaction [1]. Formic acid (HCOOH), as the elementary carboxylic acid, is proposed to occur as an intermediate during this reaction. In material science magnetite nanoparticles are linked by larger carboxylic acids to form supercrystals with exceptional mechanical properties [2]. Thus, a detailed atomic understanding of the interaction at the magnetite surface/carboxylic acid interface is vital. In this contribution the adsorption of formic acid on the magnetite (111) single crystal surface is studied under UHV conditions at room temperature. Our FT-IRRA spectroscopy results and DFT calculations show dissociative adsorption of formic acid in quasi-bidentate and chelating geometries, the latter being stabilized by the presence of tetrahedral iron vacancies at the surface. The locally observed ($\sqrt{3} \times \sqrt{3}$) R 30° superstructure by STM consists of formate in a triangular arrangement, adsorbed predominantly in chelating geometry. This contribution will present results from experiments performed at the DESY NanoLab and the European Synchrotron Radiation Facility (ESRF).

References

- [1] M. Zhu *et al.*, ACS Catalysis **6**, 722-732 (2016)
- [2] A. Dreyer *et al.*, Nature Materials **15**, 522-528 (2016)

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