



# Organic-Metal Hybrid Interfaces at the Mesoscopic Scale

Giovanni Zamborlini

Information

Band / Volume 55

ISBN 978-3-95806-328-0

Mitglied der Helmholtz-Gemeinschaft

Forschungszentrum Jülich GmbH  
Peter Grünberg Institut (PGI)  
Elektronische Eigenschaften (PGI-6)

# **Organic-Metal Hybrid Interfaces at the Mesoscopic Scale**

Giovanni Zamborlini

Schriften des Forschungszentrums Jülich  
Reihe Information / Information

Band / Volume 55

ISSN 1866-1777

ISBN 978-3-95806-328-0

# Contents

<b>Zusammenfassung</b>	<b>v</b>
<b>Synopsis</b>	<b>vii</b>
<b>Introduction</b>	<b>ix</b>
<b>1 Molecule-metal interactions</b>	<b>1</b>
1.1 Basic properties of organic-metal interfaces . . . . .	1
1.2 What determines the orbital binding energies? . . . . .	3
<b>2 Porphyrin molecules</b>	<b>7</b>
2.1 Introduction . . . . .	7
2.1.1 Structure . . . . .	7
2.1.2 Importance and applications . . . . .	9
2.2 Porphyrins on metals: surface interactions . . . . .	9
2.2.1 Adsorption geometry . . . . .	10
2.2.2 Electronic structure . . . . .	14
2.2.3 Magnetic properties . . . . .	17
2.2.4 Functionalization . . . . .	19
<b>3 Methods</b>	<b>23</b>
3.1 Photoemission spectroscopy . . . . .	24
3.2 Absorption spectroscopy . . . . .	27
3.2.1 NEXAFS . . . . .	28
3.3 PEEM . . . . .	29
3.3.1 NanoESCA microscope . . . . .	30
3.3.2 Laterally resolved XPS . . . . .	35
3.3.3 $\mu$ -ARPES . . . . .	37
3.3.4 Laterally resolved XAS . . . . .	37
3.4 LEEM . . . . .	37
3.4.1 Working principle . . . . .	37
3.4.2 SPELEEM microscope . . . . .	38
3.4.3 Contrast methods in LEEM . . . . .	39
3.5 Molecular Orbital Tomography . . . . .	40
3.5.1 The plane wave approximation . . . . .	40
3.5.2 A practical example . . . . .	41

---

3.6	Scanning Tunneling Microscopy . . . . .	44
3.6.1	Working principle . . . . .	44
3.6.2	Experimental apparatus . . . . .	46
<b>4</b>	<b>Experimental details</b> . . . . .	<b>47</b>
4.1	Sample preparation and methods . . . . .	47
4.2	Sample characterization . . . . .	48
<b>5</b>	<b>Organic semiconductors on transition metals: NiTPP/Cu(100)</b> . . . . .	<b>53</b>
5.1	Introduction . . . . .	53
5.2	Geometric structure . . . . .	53
5.2.1	Characterization of the highly oriented NiTPP self-assembly . . . . .	53
5.2.2	Adsorption geometry . . . . .	55
5.3	Electronic structure . . . . .	59
5.3.1	Periodic DFT calculations . . . . .	59
5.3.2	Valence band . . . . .	63
5.3.3	Core level spectroscopies . . . . .	69
5.4	LEEM studies of the NiTPP self-assembly . . . . .	72
5.4.1	Radiation damage of the molecular film . . . . .	72
5.4.2	Dark-field LEEM on the ordered NiTPP phases . . . . .	75
5.5	From nickel to cobalt tetraphenyl porphyrin . . . . .	77
5.6	Conclusions . . . . .	78
<b>6</b>	<b>Electronic structure of NiTPP and CoTPP on different substrates</b> . . . . .	<b>81</b>
6.1	Introduction . . . . .	81
6.2	NiTPP and CoTPP on Cu(110) . . . . .	83
6.3	NiTPP and CoTPP on Ag(110) . . . . .	87
6.4	Conclusions . . . . .	91
<b>7</b>	<b>Functionalization of NiTPP/Cu(100) by NO adsorption</b> . . . . .	<b>93</b>
7.1	Introduction . . . . .	93
7.2	LEED and STM . . . . .	94
7.3	NEXAFS, XPS and UPS . . . . .	97
7.4	Conclusions . . . . .	103
	<b>Outlook</b> . . . . .	<b>105</b>
	<b>Conclusions</b> . . . . .	<b>109</b>
	<b>Abbreviations</b> . . . . .	<b>111</b>
	<b>Publications and conference contributions</b> . . . . .	<b>115</b>
	<b>Bibliography</b> . . . . .	<b>133</b>

Information

Band / Volume 55

ISBN 978-3-95806-328-0

Mitglied der Helmholtz-Gemeinschaft

