

Interacting Interactions: A Study on the Interplay of Molecule-Molecule and Molecule-Substrate Interactions at Metal-Organic Interfaces

Martin Willenbockel

Forschungszentrum Jülich GmbH
Peter Grünberg Institut (PGI)
Functional Nanostructures at Surfaces (PGI-3)

Interacting Interactions: A Study on the Interplay of Molecule-Molecule and Molecule-Substrate Interactions at Metal-Organic Interfaces

Martin Willenbockel

Schriften des Forschungszentrums Jülich
Reihe Schlüsseltechnologien / Key Technologies

Band / Volume 99

ISSN 1866-1807

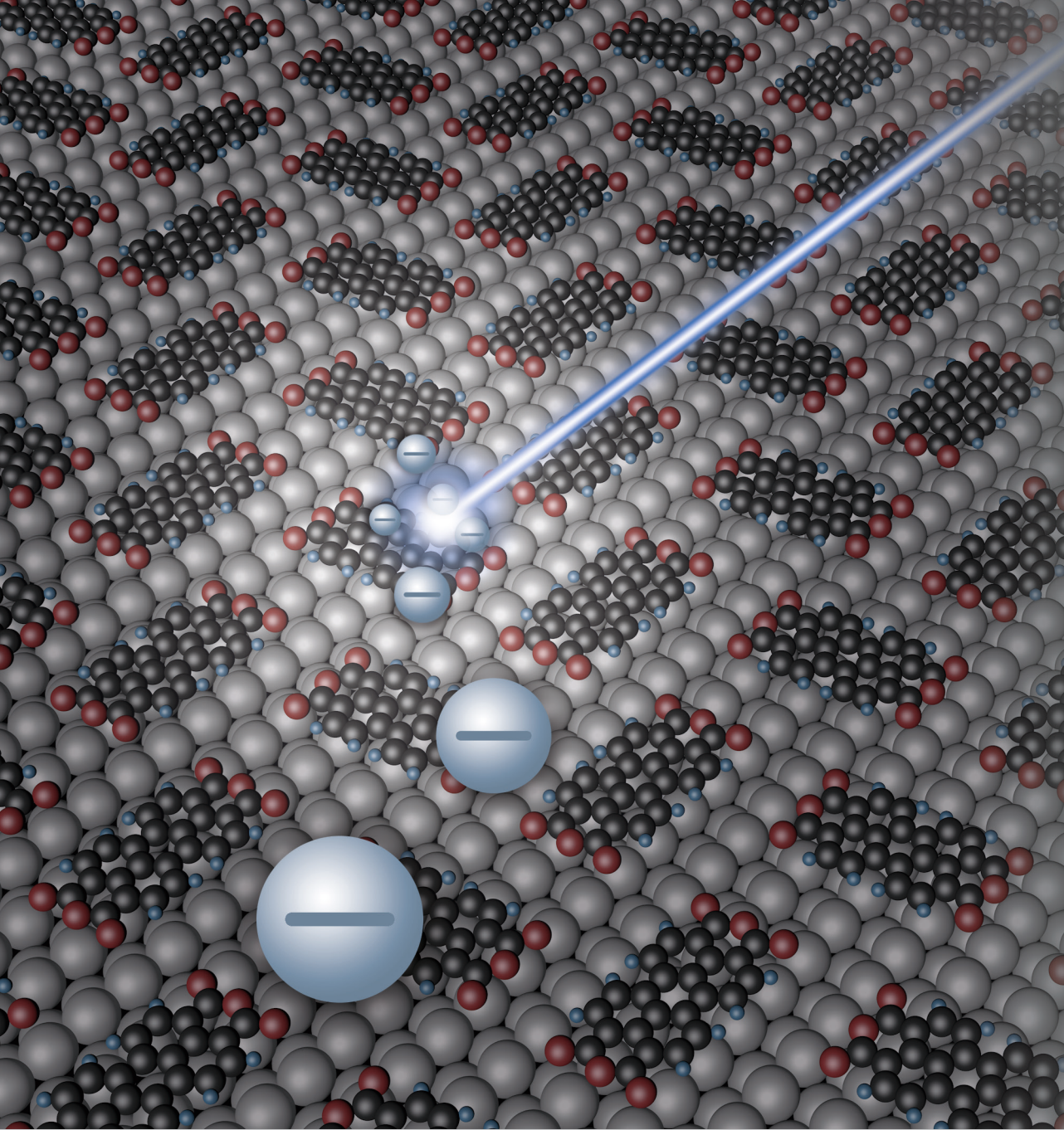
ISBN 978-3-95806-018-0

Contents

1	Introduction	1
2	Methods	5
2.1	Introduction	5
2.2	Photoelectron spectroscopy	5
2.3	Angle resolved photoelectron spectroscopy	8
2.4	X-Ray standing waves	10
2.5	Experimental setups	16
2.5.1	ARPES	16
2.5.2	XSW	17
3	Benzene on Ag(111) and Cu(111)	19
3.1	Introduction	19
3.2	Benzene on Ag(111)	20
3.2.1	Introduction	20
3.2.2	Experimental details	21
3.2.3	X-ray induced changes	22
3.2.4	Coverage estimation	25
3.2.5	XSW results	27
3.2.6	Conclusion	29
3.3	Benzene on Cu(111)	33
3.3.1	Introduction	33
3.3.2	Experimental details	34
3.3.3	Beam damage	35
3.3.4	Coverage estimation	36
3.3.5	XSW analysis	37
3.3.6	LEED	43
3.3.7	Conclusion	44
3.4	Summary	48

4 Azobenzene Cu(111)	49
4.1 Introduction	49
4.2 Submonolayer coverage regime	50
4.2.1 LEED results	50
4.2.2 XPS model	51
4.2.3 XSW analysis	53
4.3 Ordered point-on-line phase	57
4.3.1 LEED results	57
4.3.2 XPS Model	58
4.3.3 XSW analysis	60
4.4 Ordered commensurate phase	65
4.4.1 LEED results	65
4.4.2 XPS model	67
4.4.3 XSW analysis	67
4.5 Multilayer	74
4.5.1 XPS models	74
4.5.2 Coverage estimation	75
4.5.3 XSW results	78
4.6 Discussion	83
4.6.1 Introduction	83
4.6.2 Distortion of azobenzene for the DP	83
4.6.3 Coverage dependent dissociation	87
4.6.4 Ordered lateral structures	91
4.7 Conclusion	94
5 Geometric and electronic structure of PTCDA on low index Ag sur-	
faces	99
5.1 Introduction: An attempt of a comprehensive view	99
5.2 Lateral structures of PTCDA on Ag(111) and Ag(100)	101
5.3 Lateral structures of PTCDA/Ag(110)	102
5.4 Vertical structure of PTCDA/Ag(100)	104
5.4.1 Introduction	104
5.4.2 Experimental details	105
5.4.3 Coverage estimation	106
5.4.4 PTCDA/Ag(100) - C1s results	108
5.4.5 PTCDA/Ag(100) - O1s results	114
5.4.6 Adsorption site determination for PTCDA/Ag(100)	119

5.4.7	PTCDA/Ag(100) - Substrate results	123
5.4.8	Discussion	124
5.5	A/B split for PTCDA/Ag(110)	132
5.5.1	Introduction	132
5.5.2	Results	133
5.5.3	Discussion	136
5.6	Energy level alignment of LUMO and HOMO in PTCDA/Ag	140
5.6.1	Introduction	140
5.6.2	Experimental results	141
5.6.3	Discussion	142
5.7	Native order of stronger bound molecular Orbitals	148
5.7.1	Introduction	148
5.7.2	Results	149
5.7.3	Discussion	153
5.8	Summary	155
6	TPA:Fe/Cu(100) - A metal organic network	157
6.1	Introduction	157
6.2	Experimental	158
6.3	O1s results	161
6.4	Fe results	166
6.5	C1s results	172
6.6	Oxygen dosing on TPA:Fe/Cu(100)	178
6.7	Conclusions	182
7	Summary	187
A	Appendix	191
	Bibliography	225



Schlüsseltechnologien / Key Technologies
Band / Volume 99
ISBN 978-3-95806-018-0

