

Contents

1	Introduction	1
1.1	Surface Science of NO	1
1.2	Electronic States of NO Adsorbed on Metal Surfaces	2
1.3	Geometries of NO on Metal Surfaces	6
1.3.1	Dissociative Adsorption	7
1.3.2	Molecular Adsorption	8
1.3.3	NO Dimers	11
1.3.4	N ₂ O	13
1.4	Previous Investigations of NO on Coinage Metal Surfaces	14
1.4.1	NO on Ag Surfaces	14
1.4.2	NO on Au Surfaces	15
1.4.3	NO on Cu Surfaces	16
1.5	Thesis Outline	20
	References	21
2	Principles and Methods	29
2.1	Principles and Equipment	29
2.1.1	Principles of STM	29
2.1.2	Principles of RAIRS	39
2.1.3	Principles of EELS	40
2.2	Methods	41
2.2.1	STM Methods	41
2.2.2	RAIRS Methods	44
2.2.3	EELS Methods	45
2.2.4	DFT Methods	45
	References	46

3	Visualization of Covalent Bonding between NO Molecules on Cu(110)	51
3.1	Introduction	51
3.2	Results and Discussion	51
3.2.1	NO Monomers	51
3.2.2	NO Dimers	55
3.3	Summary	60
	References	60
4	NO Reduction by Co-adsorbed Water Molecules on Cu(110)	63
4.1	Introduction	63
4.2	Results and Discussion	64
4.2.1	Formation of a NO-H ₂ O Complex	64
4.2.2	Rupture of the N-O Bond by Water Molecules	68
4.3	Summary	70
	References	71
5	Thermal and Electron-Induced Configuration Changes of NO on Cu(110)	73
5.1	Introduction	73
5.2	Results and Discussion	74
5.2.1	STM Observations of NO Monomers	74
5.2.2	RAIRS Measurements of NO Monomers	74
5.2.3	EELS Measurements of NO Monomers	77
5.2.4	STM Observations of Thermal and Electron-Induced Configuration Changes	79
5.2.5	Potential Energy Diagram of NO/Cu(110)	84
5.3	Summary	85
	References	85
6	Valence Orbitals of High Symmetry NO on Cu(001)	87
6.1	Introduction	87
6.2	Results and Discussion	87
6.2.1	Adsorption of NO on Cu(001)	87
6.2.2	Reaction of NO at Cu(001)	91
6.3	Summary	93
	References	94
7	Symmetry Correlation between Molecular Vibrations and Valence Orbitals: NO/Cu(110) and NO/Cu(001)	95
7.1	Introduction	95
7.2	Results and Discussion	96
7.2.1	IETS Measurements of NO Monomers	96
7.2.2	DFT Calculations of IETS for NO Monomers	97
7.2.3	IETS of NO Dimers	101

7.3	Summary	103
	References	104
8	Formation of Unique Trimer of NO on Cu(111)	107
8.1	Introduction	107
8.2	Results and Discussion	107
	8.2.1 Adsorption Geometry of NO/Cu(111) at 6 K	107
	8.2.2 Adsorption Geometry of NO/Cu(111) at 80 K	112
8.3	Summary	114
	References	114
9	Conclusions	117
10	Appendix: Analysis of Tunneling Current Modified by Vibrational Excitations	119
10.1	Introduction	119
10.2	<i>I</i> - <i>V</i> Measurements of (OH) ₂ on Cu(110)	119
10.3	<i>I</i> - <i>V</i> Measurements of (OH) ₂ ···NH–OH on Cu(110)	123
	References	125
	Curriculum Vitae	127

Reactivity of Nitric Oxide on Copper Surfaces

Elucidated by Direct Observation of Valence Orbitals

Shiotari, A.

2017, XIII, 129 p. 66 illus., 61 illus. in color., Hardcover

ISBN: 978-981-10-4581-3