

Contents

III/42 Physics of Covered Solid Surfaces

A: Adsorbed Layers on Surfaces

Part 4: Adsorbed species on surfaces and adsorbate-induced surface core level shifts

1	Introduction to physical and chemical properties of adlayer/substrate systems (H.P. BONZEL)	see subvolume III/42A1
2	Characterization of adsorbate overlayers: measuring techniques (CH. WÖLL)	see subvolume III/42A2
3	Data: Adsorbate properties	
3.1	Adsorption of noble gases	
3.1.1	Noble gases on metals and semiconductors (P. ZEPPENFELD)	see subvolume III/42A1
3.1.2	Noble gases on graphite, lamellar halides, MgO and NaCl (M. BIENFAIT)	see subvolume III/42A1
3.2	Adsorption of alkali metals	
3.2.1	Alkali metals on metals (R.D. DIEHL, R. McGRATH)	see subvolume III/42A1
3.2.2	Alkali metals on semiconductors (E.G. MICHEL, R. MIRANDA)	see subvolume III/42A1
3.3	Adsorption of metals	
3.3.1	Metals on metals (H. BRUNE)	see subvolume III/42A1
3.3.2	Metals on semiconductors (V.G. LIFSHITS, K.OURA, A.A. SARANIN, A.V. ZOTOV)	see subvolume III/42A1
3.4	Non-metallic atomic adsorbates on metals and semiconductors	
3.4.1	Chemisorbed hydrogen on metals and semiconductors (K. CHRISTMANN)	see subvolume III/42A5
3.4.2	Adsorption of C, N, and O on metal surfaces (H. OVER)	2
3.4.2.1	Introduction	2
3.4.2.1.1	General remarks	2
3.4.2.1.2	List of acronyms	2
3.4.2.2	Oxygen adsorption on metal surfaces	4
3.4.2.2.1	The dissociative sticking coefficient of oxygen on metal surfaces and its dependence on the impact energy of the incident O ₂ molecule	13
3.4.2.2.2	The heat of adsorption of chemisorbed oxygen overlayers on metal surfaces	18
3.4.2.2.3	Oxygen-metal bond strength (ab initio calculations)	20
3.4.2.2.5	Vibrational properties of chemisorbed oxygen	30
3.4.2.2.6	Local atomic oxygen-metal geometry	33
3.4.2.2.7	Ordered overlayers of chemisorbed oxygen and surface oxides on metal surfaces	37
3.4.2.2.8	Phase diagrams and phase transitions in the O-metal surface system	40
3.4.2.3	Nitrogen adsorption on metal surfaces	41
3.4.2.3.1	The dissociative sticking coefficient of nitrogen on metal surfaces	43
3.4.2.3.2	The heat of adsorption of chemisorbed nitrogen overlayers on metal surfaces	44
3.4.2.3.3	Nitrogen-metal bond strength (ab initio calculations)	45
3.4.2.3.4	Electronic properties of chemisorbed nitrogen on metal surfaces	46
3.4.2.3.5	Vibrational properties of chemisorbed nitrogen atoms	47
3.4.2.3.6	Local atomic nitrogen-metal geometry	48
3.4.2.3.7	Ordered overlayers of chemisorbed nitrogen atoms on metal surfaces	49

3.4.2.4	Carbon adsorption on metal surfaces.....	50
3.4.2.4.1	Carbon-metal bond strength.....	51
3.4.2.4.2	Electronic properties of chemisorbed carbon on metal surfaces.....	51
3.4.2.4.3	Vibrational properties of chemisorbed carbon atoms.....	52
3.4.2.4.4	Local atomic carbon-metal geometry.....	53
3.4.2.4.5	Ordered overlayers of chemisorbed carbon atoms on metal surfaces.....	54
3.4.2.5	References for 3.4.2.....	55
3.4.3	Halogens on metals and semiconductors (E.I. ALTMAN).....	see subvolume III/42A1
3.4.4	Adsorption of S, P, As, Sb and Se on metals, alloys and semiconductors (M. ENACHESCU, M. SALMERON).....	see subvolume III/42A3
3.5	Surface segregation of atomic species (H. VIEFHAUS, H.-J. GRABKE, CH. UEBING).....	see subvolume III/42A3
3.6	Molecules on graphite, BN, MgO (except noble gases)	
3.6.1	Adsorption of molecules on MgO (J. SUZANNE).....	see subvolume III/42A3
3.6.2	Adsorption of molecular hydrogen isotopes on graphite and BN (H. WIECHERT).....	see subvolume III/42A3
3.7	Molecular diatomic adsorbates on metals and semiconductors	
3.7.1	CO and N ₂ adsorption on metal surfaces (A. FÖHLISCH, H.P. BONZEL).....	74
3.7.1.1	Introduction.....	75
3.7.1.1.1	Thermodynamic properties.....	76
3.7.1.1.2	Vibrational properties.....	77
3.7.1.1.3	Geometric structure.....	78
3.7.1.1.4	Electronic structure and adsorption models.....	80
3.7.1.1.5	Atom specific electronic structure and the allylic model of CO adsorption.....	85
3.7.1.2	CO adsorption on fcc metal surfaces.....	87
3.7.1.3	CO adsorption on bcc metal surfaces.....	102
3.7.1.4	CO adsorption on hcp metal surfaces.....	110
3.7.1.5	CO adsorption on simple cubic metal surfaces.....	120
3.7.1.6	CO adsorbed on relevant binary systems, modelled by ultra-thin metal overlayers.....	121
3.7.1.7	Adsorption of N ₂ on metals.....	124
3.7.1.8	Organization of the tables.....	135
3.7.1.9	References.....	202
3.7.2	NO, CN, O ₂ on metals (W.A. BROWN).....	see subvolume III/42A3
3.7.3	Adsorption of diatomic molecules on alloy surfaces (B. E. NIEUWENHUYS).....	see subvolume III/42A3
3.8	Molecular polyatomic adsorbates on metals and semiconductors	
3.8.1	H ₂ O and OH on metals (G. PIRUG).....	see subvolume III/42A5
3.8.2	H ₂ O and OH on semiconductors (W. JAEGERMANN, T. MAYER).....	226
3.8.2.1	Introduction.....	226
3.8.2.2	Surface preparation.....	229
3.8.2.3	Surface structure: relaxation and reconstruction.....	229
3.8.2.4	Surface electronic structure and surface potentials.....	230
3.8.2.5	Methods of investigation.....	231
3.8.2.6	Adsorption mode.....	232
3.8.2.7	Thermodynamic data of adsorption.....	234
3.8.2.8	Kinetic data of adsorption/desorption, surface diffusion and surface reactions.....	234
3.8.2.9	Local structure.....	236

3.8.2.10	Long range order	237
3.8.2.11	Electronic properties	238
3.8.2.12	Core level lines	240
3.8.2.13	Vibrational properties	241
3.8.2.14	Figures for 3.8.2	275
3.8.2.15	References for 3.8.2	296
3.8.3	Adsorbate properties of NH ₃ and PF ₃ on metals and semiconductors (E. HASSELBRINK)	see subvolume III/42A3
3.8.4	CO ₂ , NO ₂ , SO ₂ , OCS, N ₂ O, O ₃ (B.E. KOEL)	see subvolume III/42A5
3.8.5	Substituted hydrocarbons on metal surfaces (W.T. TYSOE, D.R. MULLINS)	see subvolume III/42A3
3.8.6	Linear hydrocarbons and CH ₄ on metals and semiconductors (G. SOMORJAI, G. RUPPRECHTER)	see subvolume III/42A5
3.8.7	Cyclic hydrocarbons (G. HELD, H.P. STEINRÜCK)	300
3.8.7.1	List of symbols and abbreviations	300
3.8.7.2	Benzene (C ₆ H ₆)	301
3.8.7.3	Cyclohexane (c-C ₆ H ₁₂)	303
3.8.7.4	Other saturated cyclic hydrocarbon molecules (cycloalkanes)	304
3.8.7.4.1	Cyclopropane (c-C ₃ H ₆)	304
3.8.7.4.2	Cyclobutane (c-C ₄ H ₈)	304
3.8.7.4.3	Cyclopentane (c-C ₅ H ₁₀)	305
3.8.7.4.4	Cyclooctane (c-C ₈ H ₁₆)	305
3.8.7.5	Non-saturated cyclic hydrocarbon molecules (other than benzene)	305
3.8.7.5.1	Cyclopentene (c-C ₅ H ₈)	305
3.8.7.5.2	Cyclopentadiene (c-C ₅ H ₆)	305
3.8.7.5.3	Cyclohexene (c-C ₆ H ₁₀)	306
3.8.7.5.4	Cyclohexadiene (c-C ₆ H ₈)	306
3.8.7.5.5	Cyclooctadiene (c-C ₈ H ₁₂) and Cyclooctatetraene (c-C ₈ H ₈)	306
3.8.7.6	Ethylene Oxide (C ₂ H ₄ O)	306
3.8.7.7	Pyridine (C ₅ H ₅ N)	307
3.8.7.8	List of Tables	308
3.8.7.9	Tables for 3.8.7	309
3.8.7.10	Figures for 3.8.7	354
3.8.7.11	References for 3.8.7	362
3.8.8	Oxygenated hydrocarbons on metals and semiconductors (J. VOHS) ..	see subvolume III/42A3
3.8.9	Halogen-substituted hydrocarbons on metals and semiconductors (J. FIEBERG, J.W. WHITE)	see subvolume III/42A3
3.8.10	Polyatomic chain-like hydrocarbons on metals and semiconductors (W. ECK)	371
3.8.10.1	Introduction	371
3.8.10.2	Physical and Chemical Properties	371
3.8.10.2.1	Structural data: Tilt and twist angles, packing and lattice structures	371
3.8.10.2.2	Heat of formation and thermal stability	373
3.8.10.2.3	Wettability	374
3.8.10.2.4	Anchor groups for SAMs on inorganic substrates	374
3.8.10.3	List of abbreviations	374
3.8.10.4	Tables	375
3.8.10.5	References for 3.8.10	380
3.9	Adsorption on oxides (H. KUHLENBECK, H.J. FREUND)	see subvolume III/42A5
3.11	Surface diffusion on metals, semiconductors, and insulators (E.G. SEEBAUER, M.Y.L. JUNG)	see subvolume III/42A1

4	Data: Adsorbate-induced changes of substrate properties.....	see subvolume III/42A2
4.1	Surface structure on metals and semiconductors (M.A. VAN HOVE, K. HERMANN, P.R. WATSON)	see subvolume III/42A2
4.2	Electron work function of metals and semiconductors (K. JAKOBI) ..	see subvolume III/42A2
4.3	Adsorbate induced surface core level shifts of metals (R. DENECKE, N. MÅRTENSSON)	388
4.3.1	Introduction	388
4.3.2	Data section	396
4.3.2.1	Al(001)	397
4.3.2.2	Al(111)	398
4.3.2.3	Ni(100)	398
4.3.2.4	Mo(110)	399
4.3.2.5	Ru(0001)	399
4.3.2.6	Ru(10 $\bar{1}$ 0)	400
4.3.2.7	Rh(100)	401
4.3.2.8	Rh(110)	401
4.3.2.9	Rh(111)	401
4.3.2.10	Stepped Rh surfaces	403
4.3.2.11	Pd(100)	403
4.3.2.12	Pd(110)	404
4.3.2.13	Pd(111)	405
4.3.2.14	Ta(100)	406
4.3.2.15	Ta(110)	406
4.3.2.16	Ta(111)	407
4.3.2.17	Ta (poly)	407
4.3.2.18	W(100)	407
4.3.2.19	W(110)	409
4.3.2.20	W(111)	411
4.3.2.21	W(320) and other stepped W	411
4.3.2.22	W (poly)	412
4.3.2.23	Os(0001)	413
4.3.2.24	Ir(100)	413
4.3.2.25	Ir(110)	413
4.3.2.26	Ir(332)	413
4.3.2.27	Pt(110)	414
4.3.2.28	Pt(111)	414
4.3.2.29	Stepped Pt surfaces	416
4.3.2.30	Au(100)	416
4.3.2.31	Au(110)	416
4.3.2.32	Au(111)	417
4.3.2.33	Au (poly)	417
4.3.3	References	418
4.4	Surface free energy and surface stress (D. SANDER, H. IBACH)	see subvolume III/42A2
4.5	Surface phonon dispersion (M.A. ROCCA)	see subvolume III/42A2
4.6	Surface optical properties (N. ESSER, W. RICHTER)	see subvolume III/42A5
	Erratum	422

Adsorbed Species on Surfaces and Adsorbate-Induced
Surface Core Level Shifts

2005, XVIII, 424 p. With CD-ROM., Hardcover

ISBN: 978-3-540-20281-3