

# Index

- A**
- Acetaldehyde, 43, 146, 147, 150, 295–298
- Acetylene ( $C_2H_2$ ), 2–10, 12–22
- Acetylene cyclotrimerization, 2–8, 12, 15, 17, 33
- Acetylene hydrogenation, 9, 14, 16–22
- Achiral inorganic material, 108
- Achiral molecules, 108–112
- Acid/base, 500, 504, 513, 514
- Acid/base catalysis, 500, 504–506, 514
- Acid/base cooperativity, 500, 504
- Acid/thiol catalysts, 501–502, 513, 514
- Activation energy, 1–3, 17, 33, 37, 46, 67, 176, 198, 216, 332, 354, 402, 487, 498
- Activation entropy, 196, 487
- Activation entropy for desorption, 196
- Active phase, 30, 312, 334, 387, 388
- Active sites, 14, 33, 46, 69, 133, 143, 270, 275, 276, 289, 293–295, 302, 303, 312, 327, 332, 353, 372, 374, 396, 399, 442, 443, 458, 483, 496, 500, 508, 510, 513, 515
- Adsorbate, 1, 2, 6, 47, 59, 60, 63, 66, 68, 77, 79, 83, 90, 91, 97–113, 117, 123, 124, 127–130, 133, 144, 147, 150, 175, 176, 179, 182, 185, 196, 197, 203–206, 210–213, 215, 216, 218, 224, 225, 228, 230, 242, 246, 254, 255, 257–264, 266–269, 279, 284, 285, 320, 334, 358, 368, 423
- Adsorbate orientation, 88, 93, 110
- Adsorption, 2, 33, 52, 77, 98, 118, 138, 155, 175, 206, 224, 253, 281, 302, 331, 348, 375, 400, 415, 443, 475
- Adsorption geometry, 146, 336
- Aldolase enzymes, 505
- Aldolase mimic, 504
- Aldol reaction, 503, 505, 514
- Alkali ion scattering spectroscopy (ALISS), 32, 33
- Alkenes, 3, 5, 15, 23, 38–40, 47, 142–143, 428, 487, 488
- Alloys, 29–47, 52–59, 64–66, 164, 165, 168, 170, 171, 277, 280–289, 319, 328, 361, 372, 374, 429, 466
- Allylic, 40, 263–267, 270, 464
- Alumina, 6–8, 12, 29–31, 309–311, 325, 326, 328, 347, 353, 359, 380, 500
- Aluminophosphates, 459, 461
- Aluminum oxides, 309–311, 359
- Amine/urea catalysts, 502–504, 512
- Aminosilica, 443–446
- Anions, 63, 65, 137, 300, 303, 304, 306, 308, 424
- Anisotropic 2D crystallization, 234
- Asymmetric catalysis, 458, 464, 479, 480
- Atomic layer deposition (ALD), 347, 359
- Atomic resolution, 83, 162, 236, 329
- Atom transfer radical polymerization (ATRP), 447, 448
- Auger electron spectroscopy (AES), 32, 35, 37, 40, 43, 55, 156, 164, 178, 188, 189, 379, 381
- Autocatalytic, 242–245
- B**
- Benzene, 3–16, 40–43, 267, 269, 270, 355, 356, 378, 467, 476
- Benzene ( $C_6H_6$ ), 42
- Benzyl protecting group, 445, 446
- Bifunctional catalysts, 500–506
- Bimetallic, 29–32, 35, 39, 40, 44, 46, 47, 51–70, 164, 170, 312, 321, 322, 360, 374, 415–435, 458, 466–471
- Bimetallic and trimetallic nanoparticles, 466–471
- Bimetallic oxide clusters, 312
- Bimetallic surfaces, 30, 32, 35, 53–69

- Binding energy, 54, 56, 69, 85, 122, 138,  
 139, 143, 144, 161, 209–211, 213,  
 255, 256, 260, 261, 263, 300, 301,  
 304, 337, 368, 387  
 Binding sites, 400, 401, 441, 477, 478  
 Biological catalysts, 495  
 Biomolecules, 76  
 Bisphenol A, 501, 503, 513  
 Bitartrate, 99–109, 111, 113  
 Blyholder model, 254, 262  
 $\pi$ -Bonded ethylene, 20  
 Breaking mirror symmetry, 109  
 Bulk alloys, 52–56, 58  
 Bulk oxides, 160, 170, 226, 230, 369, 370,  
 379, 388, 390  
 Butadiene, 40, 332–333, 355
- C**
- Calorimetry, 175–199  
 Carbon, 2, 37, 62, 100, 117, 160, 178, 210,  
 224, 261, 277, 299, 320, 355, 376, 397,  
 427, 450, 459, 485, 513  
 Carbonaceous deposits, 287, 335, 337  
 Carbon-carbon bond formation, 397, 398,  
 404–410, 450  
 Carbon deposition on Ni, 277, 278, 282,  
 287, 289  
 Carbon monoxide (CO), 5, 10, 11, 17, 21, 62,  
 120, 160, 178–184, 210, 224, 261, 299,  
 300, 303  
 Carbon oxidation, 278  
 Carbon-poisoned surface, 21  
 Carbon poisoning, 277, 278, 280  
 Carboxylate, 100, 105, 106, 112, 146, 150,  
 226, 242, 244, 245, 508, 510  
 Catalysis, 2, 29, 67, 77, 97, 118, 171, 175,  
 203, 247, 253, 275, 293, 319, 345, 367,  
 395, 415, 441, 458, 476, 495  
 Catalyst activation, 324, 372  
 Catalyst composition, 284, 334, 470  
 Catalyst immobilization, 442, 447  
 Catalysts, 1, 29, 52, 77, 98, 117, 133, 155,  
 181, 206, 242, 253, 276, 293, 319, 345,  
 368, 395, 415, 441, 457, 475, 495  
 Catalyst stability, 452  
 Catalyst-support interactions, 312  
 Catalyst synthesis, 285–289, 508  
 Catalytic ignition, 390  
 Catalytic metals, 223–247  
 Catalytic triad, 496–498, 508–510  
 Cationic clusters, 302, 304, 308, 349  
 Characterization, 29–47, 53–56, 58–61, 108,  
 133, 160, 285–289, 320–322, 327, 331,  
 346, 348–350, 358, 361, 369–372, 374,  
 375, 379, 388, 390, 391, 415–422,  
 427–428, 430–435, 448, 471, 515  
 Charge density difference, 257, 265,  
 268, 269  
 Charging effects, 294  
 Chemical vapor deposition (CVD), 372,  
 483, 484  
 Chemisorption, 30, 31, 33, 35–41, 47, 52, 68,  
 160, 180, 185, 186, 188–192, 194, 225,  
 226, 229, 230, 233, 257, 261, 262, 266,  
 269, 270, 423  
 Chiral, 75–93, 97–113, 458, 463–465, 479,  
 508–510, 512–514  
 Chiral acid/base, 513  
 Chiral chromatography, 78  
 Chiral distortion, 100, 106  
 Chiral silane, 514  
 Chiral transmission, 107, 108  
 Chromatography, 338, 370, 383, 387, 397  
 Clean technology, 458, 471  
 Close-packed surface, 225, 325, 401  
 Clusters, 31, 61, 117–130, 162, 164, 265,  
 268, 281, 284, 285, 293–313, 345–361,  
 409, 415–435, 458, 466, 468–471, 485,  
 486, 515  
 Coadsorption, 336  
 CO adsorption on Pd, 5, 334, 383  
 Coalescence, 82, 83, 226, 232, 326, 348, 354,  
 359, 372  
 Cobalt oxides, 306–307  
 C-O bond cleavage, 336–338  
 CO dissociation, 183, 331, 334, 337  
 CO hydrogenation, 334–337, 383, 434  
 Colloidal, 395–411  
 Concavity, 464  
 Constrained geometry-inspired catalysts  
 (CGCs), 444, 445  
 Constrained space orbital variation (CSOV),  
 257, 265  
 CO on Ni(100), 265  
 Cooperative catalysis, 496–500, 502, 503,  
 505, 515  
 CO oxidation, 142, 295, 300–305, 350–354,  
 388–391  
 Copolymerization, 445, 511  
 Copper, 105, 225–228, 269, 356, 448,  
 449, 468  
 Covalent imprinting, 506–508  
 Crotonaldehyde, 44–47, 146, 434  
 Crystal Truncation Rod (CTR), 59  
 Cu(110), 90–92, 98–106, 108–113, 225–230,  
 232, 235–237, 239, 268, 270  
 Cu<sub>3</sub>Au(100), 328, 370, 380–383

- Cu/bpy catalyst, 450  
CuBr/pyridylmethanimine (Cu/PMI), 448  
Cyclic voltammetry, 86  
Cyclohexane, 37, 42, 46, 459, 467  
Cyclohexanone, 46, 460, 513
- D**  
Dative bond, 262, 264, 271  
d-band center, 54–56, 58, 60, 64, 65, 67, 68, 119  
d-band model, 258, 259, 266  
Deactivated surfaces, 339  
Deactivation, 68, 129, 277, 278, 280, 286–288, 321, 352, 357, 448, 450  
Defects, 137–138, 143–146, 169, 189, 206, 210, 213, 234, 294, 303, 320, 321, 328, 329, 335, 351, 352, 354–356, 358, 368, 369, 382, 384, 385, 387, 390, 399, 401, 405, 406  
Dehydration, 138–142, 150  
Dehydrogenation, 29, 31, 40–43, 47, 138–142, 150, 276, 294, 336, 337, 339, 360, 371, 380, 384, 387, 471  
Density functional theory (DFT), 4, 82, 88–90, 100, 113, 123, 135, 147, 175, 178, 180, 188, 230, 256, 276, 351, 370, 418, 487  
Desorption, 3, 4, 13, 15, 20, 35, 37, 39–42, 44, 84–87, 144–146, 176, 180, 183, 184, 195–199, 204, 210–213, 225, 232, 234, 242, 244, 335, 336, 350, 351, 353, 355–357, 372, 379, 381–385, 387, 389, 406  
Desulfurization, 118, 125–130  
Dewar-Chat-Duncanson model, 254  
Dewetting, 321, 326  
Dienes, 40  
Differential heat, 177–179, 181, 182, 184–186, 188, 190  
DIMET, 204, 212  
Dimethyl gold complex, 417, 422  
Dinitrosyl species, 35, 36  
di- $\sigma$ -bonded ethylene, 19–21  
Dissociative adsorption, 35, 67, 138, 140, 183, 185, 187, 188, 190, 193, 195, 225, 260  
Doping, 312, 368  
Dynamic incorporation, 242  
Dynamic mass transport, 225, 231–232  
Dynamic nature of metal surfaces, 231  
Dynamic process, 242  
Dynamics, 203, 205, 206, 210–214, 216–219, 225, 297, 320
- E**  
Early-transition metals, 117, 118  
Electrified interfaces, 69  
Electrocatalysis, 43, 56, 61–69  
Electrocatalytic activity, 64, 65  
Electrocatalytic trends, 52, 60, 64, 69  
Electronegativity, 141, 225, 260, 312  
Electron microscopy, 169, 287, 320, 322, 326, 370–372, 375, 397, 418, 466, 470  
Electrons, 63, 136, 137, 148, 204–206, 210–213, 215–217, 254, 255, 257, 259, 260, 262, 269–271, 300, 301, 305, 384  
Eley-Ridel (ER), 302  
Enantiomer(s), 75–78, 86, 90, 91, 97, 98, 100–103, 108, 479, 480, 509, 511, 512  
Enantioselective, 75–79, 86, 87, 93, 97–99, 105, 106, 113, 158, 164, 479  
Enantioselective heterogeneous catalysis, 77, 97  
Enantioselectivity, 75–93, 97, 103, 105, 464, 479, 496, 509, 511, 512, 514, 515  
Encapsulation, 156, 160, 168–170, 321, 326, 327, 383, 443  
Energy-dispersive X-ray fluorescence, 320  
Enzyme catalysis, 496  
Enzymes, 76, 441, 458, 464, 475, 476, 489, 495–515  
Epitaxial growth, 92, 322–324  
Epitaxial thin film model catalysts, 322–327  
Ethanol, 43, 138–142, 147–150, 334, 374, 402, 405  
Ethene hydrogenation, 423  
Ethylene, 5, 7, 14, 16, 19–22, 31, 38, 39, 43, 111, 139, 143, 147, 150, 267–270, 295–299, 304, 332–333, 445, 446, 468, 509  
Ethylene hydrogenation, 5, 16, 19–22  
Ethylene oxide, 43  
Ethylidyne, 2, 3, 5, 7, 9–23  
Exchange current density, 67  
Extended x-ray absorption fine structure (EXAFS), 409, 417–433, 466, 483, 486
- F**  
Femtochemistry, 203–219  
Femtosecond, 203–205, 207, 208, 210, 218  
Fermi level, 54, 58, 64, 65, 112, 117, 124, 212, 255, 258, 260, 262, 263, 266, 267, 399  
Filtration tests, 452  
Fine chemicals, 44, 97, 459, 460, 475  
Flexible surface, 224, 245  
Fluorescence spectroscopy, 445  
Fluorinated sulfone, 446

- 2-Fold site, 33, 135, 139, 508  
 3-Fold site, 19, 33, 35, 37, 39, 69, 124, 168, 181, 184, 188, 191, 195, 206, 233, 241, 242, 338, 339  
 Formaldehyde, 43, 142–143, 146, 147, 294, 337, 338  
 Fourier transform infrared spectroscopy (FTIR), 52, 61, 327, 374  
 Friction model, 211, 212, 215  
 Frontier-orbital, 262, 264, 267  
 Functional group positioning, 495–515  
 Functioning conditions, 334  
 Furan, 143, 150
- G**  
 Ga-H formation, 374  
 Ga hydride, 372, 374  
 Gallium nitrate, 511  
 $\text{Ga}_2\text{O}_3$  model catalysts, 373  
 Gold, 57, 68, 88, 177, 184, 225, 226, 294, 299–302, 304, 309, 310, 312, 346, 349, 350, 352, 353, 359, 371, 374, 398, 399, 401, 417, 422, 423, 460, 511, 512  
 Gold catalysts, 350  
 Gold oxide, 299–302, 304  
 Grazing incidence small angle X-ray scattering (GISAXS), 358  
 Green chemistry, 319, 457–471  
 Group V metal oxides, 295  
 Guided-ion beam tandem mass spectrometer (GIB-MS), 296, 305, 309, 310
- H**  
 Half-hydrogenated, 483, 486, 487  
 Heat of adsorption, 2, 5, 176–195, 197, 198  
 Heck coupling reaction, 451  
 Height contour, 323  
 Heteroepitaxial growth, 92  
 Heterogeneous, 1, 29, 46, 77, 78, 97–99, 105, 113, 133, 156, 175, 203, 226, 247, 253, 254, 276, 277, 289, 293–313, 319, 321, 332, 339, 368, 384, 395–411, 416, 441–453, 457–471, 475, 495–515  
 Heterogeneous active site, 105  
 Heterogeneous catalysis, 77, 97, 175, 203, 247, 253, 254, 276, 277, 289, 293, 294, 296–305, 311, 312, 332, 339, 368, 384, 395–398, 410, 441–453, 499, 504  
 Heterogeneous catalysts, 1, 29, 46, 77, 113, 156, 276, 289, 293–313, 319, 321, 396, 397, 410, 416, 441, 442, 447, 457–471, 475, 495–515  
 High pressure cell, 325, 331  
 High pressure reaction cell, 331  
 High-pressure x-ray photoelectron spectroscopy (HP-XPS), 334, 336, 338, 388  
 High resolution electron energy loss spectroscopy (HREELS), 35, 36, 41–44, 122, 237, 381, 384  
 High resolution transmission electron microscopy (HRTEM), 322–325, 327, 329, 332, 370, 375, 376, 378, 387, 388, 403  
 Homogeneous, 1, 77, 97, 113, 211, 223, 295, 328, 376, 395–411, 441–453, 458, 460, 464, 471, 498, 499, 501, 503, 504, 512, 513  
 Homogeneous catalysis, 77, 395, 396, 399, 441–453, 498, 504  
 Hopping, 82, 215–217, 257, 258  
 Horiuti, J., 2, 16, 17, 20  
 Hydrocarbon, 1–23, 31, 37–44, 47, 118, 125, 142, 150, 175, 254, 262, 266–271, 277, 279, 285, 295, 303, 321, 334, 371, 372, 387, 429, 434  
 Hydrocarbon conversion catalysis, 2  
 Hydrocarbon transformation, 118  
 Hydrodesulfurization, 118, 120, 125, 128  
 Hydrogen ( $\text{H}_2$ ), 2, 9–21, 23, 37, 45, 53, 57, 59, 61–63, 67–69, 86, 101, 103, 109, 111, 112, 125, 129, 137, 140, 142–144, 146, 147, 150, 155, 208, 224, 225, 232–235, 247, 258, 270, 271, 277, 279, 321, 324, 326–327, 332, 335–337, 355, 357, 359, 368, 374, 423, 428, 434, 443, 444, 459, 460, 462, 464, 496, 502, 503, 505, 506, 510  
 Hydrogen adsorption, 16, 37, 224, 232, 258, 336  
 Hydrogenation, 2, 5, 7, 9, 11–23, 29, 31, 44–47, 77, 87, 98, 105, 106, 127–129, 276, 331–337, 372, 383, 423, 428, 434, 464, 465, 467–471, 479, 480, 483, 485, 487, 488  
 Hydrogenation of  $\beta$ -ketoesters, 77, 98, 106  
 Hydrogen bonding, 101, 103, 111, 443, 444, 496, 502, 503, 505, 506, 510  
 Hydrogen evolution reaction (HER), 62, 63, 68  
 Hydrogen-induced reconstructions on metal surfaces, 232–235

Hydrogenolysis, 44, 130, 155, 325, 423, 434  
Hydrogen oxidation reaction (HOR), 62, 63, 67, 68

## I

Immobilized palladium pincer catalysts, 451  
Immobilized polymerization catalysts, 442–450  
Imprinting, 90, 91, 444, 475, 476, 478–489, 506–511  
Incorporation of metal atoms, 223, 226, 231, 232, 239, 247  
Infrared (IR), 150, 207, 208, 333, 336, 356, 374, 417, 418, 421–424, 428  
Infrared absorption, 88, 384  
Inhibitors, 483, 485, 515  
In<sub>2</sub>O<sub>3</sub>, 367, 371, 374–377, 390  
In<sub>2</sub>O<sub>3</sub> films, 371, 374–377  
In-situ spectroscopy, 328, 333–334  
Integral heat, 177, 178, 183, 184, 186, 190, 193, 195  
Interface sites, 321, 332  
Interfacial energy, 326  
Intermolecular coupling, 147, 336  
Intermolecular hydrogen bonding, 111, 444  
Ionic charge state, 295, 301–304, 313  
Iridium catalysts, 295, 323, 357, 428  
Iron, 182, 195, 302–305, 309, 312  
Iron oxides, 302–305, 312  
Irreducible supports, 309, 310  
Isobutene, 38  
Isolated amine groups, 444

## K

Kinetic explosion, 226, 242, 244  
Kinetics, 1–3, 7, 11, 12, 15, 17, 18, 21–23, 30, 36, 38, 61–64, 66, 69, 84–86, 188, 226, 242, 247, 296, 297, 299, 300, 313, 319, 353, 398, 415, 416, 452, 471

## L

Langevin, 298  
Langmuir-Hinshelwood, 301, 302  
Langmuirian adsorption, 47  
Laser-induced thermal desorption, 4  
Leached palladium, 452, 453  
Leaching, 397, 399, 406–410, 442, 443, 449, 452  
Ligand, 33, 47, 77, 78, 117–119, 127, 129, 143, 241, 402, 404, 406, 409, 415–417,

421, 423, 424, 428–430, 435, 448–451, 464, 465, 469–471, 478–483, 486, 487

Ligand effects, 33, 47, 117–119, 127, 129  
Line defects, 328  
Lone pair, 146, 147, 254, 263, 264, 266, 270–271, 300, 301  
Low-coordination sites, 329  
Low energy electron diffraction (LEED), 4, 19, 32–35, 37, 46, 53, 55, 58, 59, 82, 93, 99, 101, 102, 106, 109–111, 136, 137, 156–158, 163, 178, 179, 182, 185, 186, 188, 189, 195, 224, 225, 230, 233, 237, 242, 243, 247, 331, 380, 381, 384  
Low energy ion scattering (LEIS), 32, 33, 35, 53–55, 57, 58, 156, 163

## M

Madelung potential, 139, 141  
Magnetic nanoparticles, 453  
MAS-NMR, 483, 484  
Mass-selected clusters, 296, 346, 348  
Materials gap, 320, 332  
Mercury poisoning tests, 452  
Mesoscopic restructuring of surfaces, 226, 230  
Metal, 2, 29, 52, 76, 98, 117, 134, 155, 176, 203, 223, 253, 277, 295, 319, 345, 367, 396, 415, 441, 464, 476, 496  
Metal carbides, 117–130, 287  
Metal-complex, 476, 479–482, 488, 489  
Metallic, 1–23, 44–46, 69, 124, 162, 168, 213, 242, 258, 276, 277, 324, 337, 338, 356, 368, 381, 384, 387–389, 396, 397, 401, 404, 406, 409, 411, 415–435, 452, 466, 469  
Metalloicyclic species, 3  
Metal nanoparticles, 162, 170, 319–340, 368, 371, 380, 395–411  
Metal oxide, 133–150, 155–171, 293–313, 323, 326, 327, 345, 347, 348, 358, 367–370, 380, 388, 407, 416–435, 511  
Metal-oxide interactions, 155–171  
Metal phosphides, 118, 125  
Metal-support interaction, 326–327, 352, 382, 383, 430, 435  
Methane activation, 279  
Methane combustion, 387, 388  
Methanol, 43, 285, 294, 295, 331, 334, 336–339, 372, 374, 376, 384, 391, 398, 400  
Methanol decomposition, 337, 338  
Methanol steam reforming, 372, 374, 376, 377  
Methylaluminoxane (MAO), 446  
Methyl methacrylate, 447, 448

- MgO, 277, 294, 328, 348, 350–352, 354, 355, 357, 358, 370, 379, 422–424, 427, 428, 434
- Michael addition, 499, 505, 512
- Microfacet, 80–82, 91, 179
- Microreactor, 44–46, 323, 370, 371, 374
- Microstructural changes, 323, 325, 334, 339
- Miller index, 75, 76, 79–84, 92, 93, 135, 176, 179, 180, 185, 186, 224, 320, 323–325
- Miller index facets, 320, 323, 324
- Missing and added row restructuring, 230
- Model catalysts, 3, 31, 44–47, 155–171, 282, 320–339, 345, 346, 348, 371, 373, 375–390, 397
- Molecular adsorption, 36, 124, 127, 190, 192–195
- Molecular beams, 4, 160, 176–178, 184, 189, 337, 354, 356, 357, 359, 389, 390
- Molecular catalysts, 416, 424, 435
- Molecular imprinting, 475–489, 507
- Molecularly-imprinted catalyst, 475–479, 486
- Molecular precursors, 416, 466
- Molecular simulation, 82, 83, 88, 93
- Molybdenum, 16, 295
- Monolayer, 4, 5, 7, 35–38, 40–44, 46, 56, 57, 62, 69, 99, 109, 137, 144, 157, 161, 164, 170, 175, 177, 181, 207, 230, 231, 328, 347, 349, 387, 483, 511, 512
- Mononuclear, 32, 416–424
- Monte Carlo, 82, 88, 105, 182, 285
- Morphologies, 324
- Multifunctional cooperativity, 498
- N**
- N adsorbed on Cu, 260
- Nanocatalysis, 396, 397, 405, 411
- Nanochannels, 105
- Nanoclusters, 162, 459, 466, 469–471
- Nanocrystals, 162, 326, 375, 460
- Nanometer-sized islands, 235, 246
- Nanometer-sized pits, 235, 246
- Nanoparticles, 64, 67, 118, 119, 156, 157, 159–162, 164, 170, 171, 302, 303, 319–340, 350, 355, 357, 358, 367–391, 395–411, 453, 458, 466–470
- Naturally chiral surfaces, 77–79, 81, 90–93
- Newns-Anderson model, 257
- Ni(110), 54–56, 66, 106–108, 113, 224, 225, 232–235, 242–245
- Ni alloys, 66, 280, 288
- Ni catalysts, 77, 98, 278, 288
- Nickel, 106, 126, 180, 186, 225–227, 265, 302, 305, 307, 308
- Nickel oxides, 307–309
- NiO(111), 382
- Nitric oxide (NO), 190–195
- Nitrogen (N<sub>2</sub>), 57, 135, 191, 195, 210, 232, 247, 254, 255, 260, 261, 263, 264, 287, 304, 356, 448, 458, 460–464
- Nitrogen oxide (NO), 35–37, 43, 190–195, 197, 205, 206, 209–213, 266, 356
- Noble, 2, 21, 117–119, 171, 258, 260, 266, 271, 296, 319–340, 348, 368, 379, 382, 387, 388, 429, 430, 434, 435
- Non-covalent imprinting, 508–511
- N<sub>2</sub> on Ni(100), 263
- Nuclear magnetic resonance (NMR), 6–8, 418, 427, 428, 448, 460, 483, 484, 506, 515
- Nucleation, 157, 185, 186, 189, 226, 232, 278, 280–282, 327, 328, 512
- Nucleation density, 328
- O**
- Octane, 271
- o*-phthalaldehyde, 508
- Organisational chirality, 100, 102
- Organocatalyst, 499, 512
- Oscillatory behavior, 390
- Overpotential deposited hydrogen (H<sub>opd</sub>), 67–69
- Oxidation, 30, 31, 44–46, 57, 62, 67–69, 86, 108, 121–123, 134, 136–139, 142–144, 149, 150, 156, 161, 162, 170, 185, 186, 189, 190, 226, 230, 276–278, 280–282, 294–296, 298–310, 312, 313, 324–328, 331, 337–339, 346, 350–355, 368, 369, 372, 374, 376–379, 381, 384, 388–391, 400, 402, 422, 434, 435, 452, 458–460, 462–464, 505
- Oxidative coupling, 143, 150, 380
- Oxide model systems, 370
- Oxides, 117, 134, 135, 139, 141, 142, 150, 164, 170, 190, 225, 226, 230, 295, 302–304, 306–313, 319–321, 367–372, 374, 376, 378–380, 382, 384, 387–391, 415–435, 458, 459, 511
- Oxygen (O<sub>2</sub>), 43–44, 47, 53, 62–67, 78, 79, 100, 106, 111, 112, 118, 121–125, 128, 133–150, 157, 164, 168, 169, 178, 184–192, 195, 224–232, 236, 237, 239, 240, 242, 246, 260, 261, 264, 266, 271, 295–298, 300–304, 306–311, 323, 327, 337, 350–354, 356, 368–370, 374, 375, 380, 381, 384, 385, 387–390, 417, 418, 420–422, 426, 428–430, 435, 458–460, 466

- Oxygen-induced reconstruction of metal surfaces, 226–232
- Oxygen reduction reaction (ORR), 53, 62–69
- Oxygen reservoir, 381, 390
- Oxygen vacancies, 139, 150, 169, 327, 368, 369, 374, 375, 384, 385, 387, 390
- P**
- Palladium (Pd), 2–8, 12, 16–19, 22, 225, 339, 396, 404–409, 450–453, 459
- Palladium catalysts, 4, 17, 404, 450–453
- Palladium pincer complexes, 451
- Partially oxidized, 337, 390
- Particle edges, 324, 334–336
- Particle shape, 329, 335, 398, 401–404
- Particle size, 64, 300, 322, 323, 326, 327, 332, 333, 338, 345, 346, 348, 350, 358, 398–400, 404–407, 452
- Particle size dependence, 332, 398–400
- Particle size effects, 332
- Pd films, 57–58, 61, 68, 156–159, 162, 164
- Pd-Ga alloys, 372, 374
- Pd-hydride, 335, 336
- Pd nanoparticles, 157, 159–161, 170, 324, 328, 329, 332, 334–336, 338, 355, 357, 382, 390, 405, 407, 409
- PdO bulk oxide, 388
- Pd<sub>5</sub>O<sub>4</sub> surface oxide, 388
- Pd-oxide phases, 337
- Pd(0)-Pd(II) catalytic cycle, 453
- Pd(II)-Pd(IV) catalytic cycle, 451
- Pd surface oxides, 388
- Pd/TiO<sub>2</sub>, 159
- Pharmaceuticals, 76, 77, 97, 447, 458, 460–464, 515
- Phonons, 204–206
- Phosphorous, 451
- Photocatalysis, 147–150
- Photoemission, 56, 121, 122, 254, 255
- Photo-oxidation, 149, 150
- Photo-reaction, 147
- Pinning, 358
- Platinum, 57, 67, 179, 196, 206, 224–226, 364, 398–400, 402, 403, 406, 416, 429, 430, 469
- Point chirality, 100–101
- Poisoning, 125, 277, 278, 280, 282, 355, 357, 390, 452
- Polanyi, M., 2, 16, 17, 20
- Polarization modulation infrared reflection absorption spectroscopy (PM-IRAS), 331
- Polyalkene hydrogenolysis, 423
- Polyethylene glycol, 512
- Polymer electrolyte membrane fuel cell (PEMFC), 53
- Polymeric poison, 452
- Polymerization of ethylene, 445, 446
- Polymorphic system, 99, 106
- Potential of zero charge (pzc), 64
- Predictive catalysis, 275
- Pre-exponential factor, 85, 176, 195–199
- Pressure gap, 16
- Propane, 277, 278, 286, 287, 350, 360, 369, 384, 386, 387
- Propene, 360, 384, 386, 387, 428, 429, 487
- Protein, 76, 496, 504, 511
- Proton-transfer, 505
- Pseudomorphic, 57, 58, 61, 68
- Pt-Al<sub>2</sub>O<sub>3</sub>, 322, 323
- Pt-skeleton, 54, 58, 59, 64, 65
- Pt-skin, 53–55, 58–60, 64–66
- Pt-Sn, 29–48, 468
- Pt/TiO<sub>2</sub>, 162–163
- Pulsed laser deposition, 92
- Q**
- Quartz, 77–79, 90, 92, 287, 323, 371
- R**
- Racemic, 76, 77, 85, 86, 88, 89, 112
- Radical, 63, 150, 254, 259–262, 264, 266, 267, 269, 270, 295, 296, 447, 448, 509
- Radical cation, 295, 296
- Randomly distributed catalysts, 501
- Rate constant, 12–14, 42, 63, 123, 124, 149, 298, 397, 511
- Rate normalization, 332
- Rational catalyst design, 276, 289, 415, 435, 471
- Reactant, 2, 16, 18, 23, 78, 98, 99, 105, 106, 113, 129, 133, 224, 253, 275, 298, 299, 305, 307–312, 354, 356–358, 396, 397, 402, 403, 406, 407, 424, 429, 447, 453, 457, 458, 465, 476, 481, 483, 485, 487, 496, 498, 499, 505, 506
- Reaction intermediate, 4, 62–64, 69, 150, 217, 218, 223–247, 429, 460, 479
- Reaction rate, 12, 17, 21, 40, 62, 150, 155, 223, 247, 285, 298, 326, 332, 354, 390, 395, 397–401, 405, 406, 410, 480, 487
- Reactor studies, 44–46, 370
- Reconstruction, 52, 53, 59, 82, 106, 108, 113, 137, 169, 175, 179, 180, 188, 189, 224–235, 247, 320

- Recoverable immobilized catalysts, 442  
 Recrystallization, 326  
 Recyclable polymerization catalyst, 447  
 Redox, 171, 376, 397–404, 459, 460, 462, 463  
 Reducible oxide, 326  
 Reducible supports, 155, 309, 310, 321  
 Reduction, 40, 46, 53, 62–67, 83, 136, 150,  
   155, 160, 164, 169, 170, 210, 224, 230,  
   271, 304, 324–327, 372, 374, 376, 378,  
   379, 385, 388, 390, 398–402, 405, 415,  
   424, 448, 479, 487, 498, 505, 514  
 Reflection-absorption infrared spectroscopy, 5  
 Reforming, 2, 29–31, 47, 277–279, 282,  
   285–288, 372, 374, 376, 391, 429, 471  
 Regeneration procedure, 442, 450  
 Relaxation, 52, 82, 205, 224, 320  
 Restructuring, 107, 224–231, 234–236, 239,  
   241, 245, 284, 285, 321, 324–325  
 Rh dimer, 485–489  
 Rhodium, 181, 225, 226, 326, 421, 486  
 Rhodium dicarbonyl, 421  
 Rotational motion, 217, 218  
 Roughening, 82–84, 226, 336
- S**
- Sabatier Principle, 64  
 Saturated hydrocarbons, 254, 262, 266–271  
 Scanning tunneling microscopy (STM), 4,  
   32, 34, 52, 59, 61, 82, 83, 90–92,  
   101–103, 105–107, 109–112, 134,  
   136, 137, 147, 156–159, 162–164,  
   167, 169, 170, 186, 204, 225–242,  
   244, 245, 247, 327–329, 332, 348,  
   349, 370, 379–382, 384, 388, 389  
 Selected area electron diffraction (SAED),  
   323–325, 370, 373, 375–379  
 Selective hydrogenation, 29, 31, 47, 98, 434,  
   469–471, 488  
 Selective oxidation, 296, 350, 369, 376,  
   459–460, 462–463  
 Selectivity, 30, 31, 35, 40, 42–47, 141,  
   156, 223, 275, 276, 280, 294, 309,  
   319, 324, 332, 334, 337, 339, 355,  
   360, 374, 376–378, 395, 415, 434,  
   435, 441, 442, 458–460, 462–464, 466,  
   467, 469, 470, 476, 479, 481, 482, 489,  
   496, 501, 507, 513  
 Self-organisation, 101  
 Separation, 77, 78, 86, 97, 127, 254, 255, 269,  
   283, 410, 443, 453, 475, 476, 499  
 Serial reaction pathway, 63  
 Serine proteases, 496, 497
- Shape, 64, 67, 68, 107, 122, 128, 185, 188,  
   189, 212, 216, 234, 263, 321, 323, 326,  
   328, 329, 335, 359, 374, 376, 379, 397,  
   398, 400–404, 406, 457, 458, 475, 476,  
   478, 479, 482, 483, 485, 487, 488, 506,  
   507, 515  
 Shape-selective, 457, 458, 478, 482, 485, 488  
 Silica, 126, 336, 350, 359, 360, 416,  
   418, 423, 443–446, 448–451, 453,  
   464–470, 476, 483, 486, 499–501,  
   503–509, 511, 513, 514  
 Silica frameworks, 499  
 Silicatein, 511  
 Single crystal, 1, 30, 52, 82, 98, 117, 133,  
   156, 175, 209, 226, 320, 345, 370,  
   416, 441  
 Single-site catalysts, 442, 459–460, 466,  
   468, 470  
 Sintering, 321, 348–350, 352, 357–359,  
   383, 469  
 SiO<sub>2</sub> overlayers, 483, 486  
 Site-blocking, 34, 47  
 Site specificity, 442  
 Site statistics, 329, 332  
 Size, 30, 32, 34, 37, 44, 47, 57, 64, 113,  
   157–159, 162, 163, 234, 278, 294, 296,  
   300, 302, 304, 312, 313, 320–323,  
   325–329, 332, 333, 338, 339, 345–361,  
   372, 382, 397–401, 404–409, 418, 429,  
   443, 444, 449, 452, 464, 465, 475, 487,  
   488, 499, 507  
 Size effects, 332, 346, 361, 429  
 Size-selected clusters, 345–361  
 Sn/Pt(100), 31–36, 41  
 Sn/Pt(111), 31–35, 37–40, 42–46  
 Soft landing, 347–349  
 Sol-gel, 478, 482, 501, 507  
 Solid oxide fuel cell (SOFC), 277, 278,  
   285, 434  
 Solution-phase, 295, 395, 396, 398, 405, 411  
 Solvent effect, 504–506  
 Sonogashira coupling reaction, 451  
 Spectroscopic methods, 328, 379, 416, 418  
 Spin-uncoupling, 258, 269  
 Static surface structures, 225  
 Steam reforming, 277–279, 282, 285–288,  
   372, 374, 376, 391  
 Step, 2, 3, 6, 16–18, 20, 23, 33, 42, 63, 67,  
   80–88, 90, 103, 104, 109, 112, 127,  
   129, 130, 136, 139, 140, 148, 170,  
   179–181, 184–186, 188, 190–194, 205,  
   206, 209–218, 230, 234–237, 241, 244,  
   245, 253, 257, 267, 275, 276, 279, 280,  
   285, 295, 300, 302, 313, 320, 321, 326,



- 328, 329, 332, 333, 335–337, 339, 348, 356, 368, 384, 385, 387, 418, 423, 424, 448, 458–463, 466–471, 486, 487, 500, 506–508
- Stepped surface, 176, 178, 180, 187, 206, 270, 323, 335
- Stereographic projection, 80, 81, 85, 101
- Stereospecific hydrogenation, 98
- Steric repulsions, 103
- Sticking probability, 37, 160, 161, 170, 176–196, 230
- Stoichiometry, 35, 40, 137, 143, 162, 163, 168, 169, 190, 228–231, 236, 247, 296, 302–304, 308, 310–313, 372, 381
- Stranski-Krastanov, 57, 61
- Strong metal support interaction (SMSI), 155–171, 321
- Structure, 4, 29, 52, 75, 99, 118, 133, 156, 178, 206, 223, 253, 276, 294, 320, 349, 368, 398, 415, 442, 458, 475, 495
- Structure-activity correlations, 323, 327, 371
- Structure-function relationship, 52, 320
- Structure-insensitive reaction, 332
- Structure of reaction intermediate, 223–247
- Structure-reactivity relationships, 296, 300
- Succinic acid, 98, 100, 108–113
- Sulfate ( $\text{SO}_4$ ), 239
- Sulfite ( $\text{SO}_3$ ), 236, 239
- Sulfonic acid support/activator, 446
- Sulfonion species, 501
- Sulfur, 118, 120, 125, 127, 128, 225, 232, 236, 247, 278, 282, 451, 458
- Sulfur dioxide, 120
- Sulfur poisoning, 125
- Sultone, 446, 513, 514
- Sum frequency generation (SFG), 16, 204, 206–208, 214, 215, 217, 218, 331, 333–338, 381–383
- Superoxide, 306, 309
- Support, 23, 30, 43, 121, 134, 155, 158, 164, 169, 170, 186, 267, 277, 285, 296, 300, 303, 305–307, 309, 310, 312, 320, 321, 326–329, 336, 345–350, 352–355, 358, 359, 368, 370, 379, 380, 382, 383, 390, 396, 397, 406, 407, 410, 416–418, 421–424, 427–430, 434, 435, 442, 446–450, 452, 453, 464–466, 469, 470, 478, 479, 484, 496, 499, 500, 506, 512
- Supported metal clusters, 423–245, 428–430
- Supported metal complexes, 416, 421
- Support effects, 326, 345, 353
- Support oxygen atoms, 417, 418, 421, 422
- Supramolecular assemblies, 105
- Surface, 1, 29, 52, 75, 97, 117, 133, 155, 175, 203, 223, 253, 278, 293, 320, 345, 367, 396, 416, 442, 457, 481, 495
- Surface alloys, 29–47, 52, 56–58, 281, 282, 285–287
- Surface complex, 226, 232, 236, 247, 423, 483
- Surface defects, 206, 368, 384, 385, 405
- Surface diffusion, 170, 204, 354
- Surface energy, 57, 58, 134, 135, 137, 361, 401
- Surface enrichment, 53
- Surface-mediated synthesis, 423, 424
- Surface oxide(s), 225, 226, 230–232, 324, 326, 387–390
- Surface oxide formation, 225, 230, 231, 388
- Surface reaction kinetics, 242
- Surface segregation, 52, 53, 57, 61
- Surface-sensitive methods, 328, 368
- Surface site statistics, 329, 332
- Surface structure, 32, 33, 52, 56, 59, 64–66, 77, 79, 82, 86, 90, 92, 133–135, 137, 192, 224, 225, 253, 266, 321, 326, 329, 336, 369, 381, 384, 418
- Surface X-ray scattering (SXS), 52, 59–62, 66
- Sustainable, 113, 457–471
- Suzuki coupling reaction, 405, 451
- Symmetry, 64, 75, 78, 79, 81, 82, 100, 102, 106, 109, 196, 207, 255, 256, 262–267, 269, 381, 421
- Synthesis, 3, 44, 76, 90–93, 118, 133, 218, 247, 285–289, 296, 319, 346, 368, 372, 380, 390, 395, 402, 416–418, 423–427, 429–430, 442–444, 448, 458, 460, 464, 475, 476, 478, 479, 482, 489, 504, 505, 508, 509, 511, 513

## T

- Tartaric acid, 77, 98–109, 113, 514
- Temperature programmed desorption (TPD), 3, 4, 13, 15, 16, 20, 35, 37, 38, 40–44, 84, 85, 127, 144–146, 150, 179, 182, 193, 198, 331, 336, 337, 350, 379, 381–387
- Temperature programmed reaction, 226, 243, 350
- Temperature programmed reaction spectroscopy (TPRS), 226, 235–237, 239, 242, 243, 247
- Template, 106, 475–483, 485–488, 506–508
- Templated chiral surface, 78, 79, 90
- Terrace, 33, 34, 80, 81, 84, 85, 90, 170, 179–181, 184–186, 188, 191, 193, 205, 206, 209–215, 217, 218, 228–230, 235–240, 246, 328, 329, 332, 336, 348, 356, 381, 382, 385, 400, 401

- Tethering, 78, 443, 464  
 Thin films, 57, 62, 168, 170, 347, 370, 371,  
     376, 380–387, 416  
 Thin Nb<sub>2</sub>O<sub>5</sub> films, 381  
 Thin oxide films, 164, 319–340, 367–391  
 Thiophene, 119, 120, 125–127, 129, 130  
 TiO<sub>2</sub> (titania), 133–150, 155–164, 167–171, 323,  
     326–327, 348–350, 352, 353, 358, 369,  
     371, 374, 378, 380, 384, 390, 422, 424  
 TiO<sub>2</sub> films on Pt, 168  
 Titanium, 134, 138–147, 150, 156, 164, 169, 309  
 Titanium dioxide, 134  
 Topographic restructuring, 239  
 Transfer hydrogenation, 479, 480  
 Transition, 2, 15, 17, 40, 47, 52, 58, 67, 98,  
     99, 117–119, 123–125, 130, 134, 185,  
     186, 196, 197, 207, 217, 218, 224, 245,  
     253, 254, 257, 258, 260–262, 266, 268,  
     271, 295, 296, 302–303, 305–312, 319,  
     334, 349, 351, 359, 368, 388, 390,  
     395–411, 416, 423, 448, 464, 479, 480,  
     498, 506, 508, 509  
 Transition metal oxides, 134, 302–303,  
     305–312, 368  
 Transition state, 124, 196, 197, 217, 218, 245,  
     253, 268, 351, 448, 479, 480, 498, 506,  
     508, 509  
 Transition state theory, 124, 196  
 Translational motion, 217  
 Transmission electron microscopy (TEM),  
     156, 277, 286–289, 320, 322, 323, 326,  
     327, 337, 370, 372, 374, 375, 377, 378,  
     397, 407, 408, 418, 427, 470  
 Trimerization, 355  
 Trityl-spaced aminosilica, 444, 445  
 Turnover frequency (TOF), 3, 207, 210, 325,  
     332, 333, 337, 354, 357, 390, 395, 398,  
     405, 483, 485, 487, 488
- U**  
 UHV chamber, 37, 176, 177, 207  
 Ultra high vacuum (UHV), 30, 51, 52, 98, 134,  
     156, 176, 230, 328, 348, 370, 379  
 Ultraviolet photoelectron spectroscopy (UPS),  
     33, 35, 42, 43, 54, 56, 60, 138, 237,  
     254–256  
 Underpotential deposited hydrogen (H<sub>upd</sub>),  
     59–61, 63, 65, 68, 69  
 α, β-Unsaturated aldehyde, 31, 44  
 Unsaturated hydrocarbon (s), 253, 254, 266–270  
 Uranium dioxide (UO<sub>2</sub>), 136, 142–147, 150  
 Uranium trioxide (UO<sub>3</sub>), 136, 142, 143, 150  
 Urea functionality, 503
- V**  
 Vanadium, 294, 295, 379, 384, 385  
 Vanadium oxides, 296–299, 378,  
     379, 384  
 Vanadium oxide thin film model  
     catalyst, 378  
 Vanadium termination, 369, 384  
 Vanadyl, 368, 369, 379, 384, 385, 387  
 Vanadyl groups, 368, 385, 387  
 Vanadyl termination, 369  
 Vibrational spectra, 333, 334, 338  
 Vibrational spectroscopy, 39, 52, 213, 247,  
     331, 381, 384  
 Vinylidene, 3–19, 23  
 Vinylidene-to-ethylidyne, 12, 17  
 Vitamins, 458, 460  
 V<sub>2</sub>O<sub>5</sub>, 379, 380, 384, 390  
 V<sub>2</sub>O<sub>3</sub> films, 378, 384  
 V<sub>2</sub>O<sub>5</sub> needles, 378, 379
- W**  
 Water dissociation, 144–146  
 Water-gas shift, 277–279, 369, 374, 376, 391  
 Weak-beam dark-field, 322, 323, 375–377  
 Well-defined, 31, 32, 46, 63, 69, 121, 124,  
     126, 162, 163, 210, 282, 320, 323, 328,  
     376, 384, 396, 415–435, 443, 446, 448,  
     450, 466, 515  
 Wetting, 321, 326
- X**  
 X-ray absorption near edge spectroscopy  
     (XANES), 417, 418, 422  
 X-ray absorption spectroscopy (XAS), 255,  
     260, 261, 271, 470  
 X-ray emission spectroscopy (XES), 254–257,  
     260, 261, 263, 267, 269, 271  
 X-ray photoelectron diffraction, 88,  
     101, 164  
 X-ray photoelectron spectroscopy (XPS), 32,  
     33, 35, 46, 125, 126, 128, 129, 136,  
     138, 139, 142, 147, 148, 156, 161, 164,  
     182, 226, 235–237, 239, 244, 247, 286,  
     287, 331, 334, 335, 337, 339, 349, 357,  
     370, 372, 379, 381, 384, 386, 387, 389,  
     390, 409
- Z**  
 Zeolite NaY, 421, 425, 426, 430, 431, 433  
 Zeolites, 374, 415–435  
 Zeolite Y, 421