References

Albrecht, T.R., Dovek, M.M., Lang, C.A., Grutter, P., Quate, C.F., Kuan, S.W.J. *et al.* (1988) *J. Appl. Phys.* **64**, 1178.

Allegretti, F., Polcik, M. & Woodruff, D.P. (2007) *Surf. Sci.* **601**, 3611.

Altman, M.S. (2010) *J. Phys.: Condens. Matter* **22**, 084017.

Alvey, M.D. & Yates, J.T., Jr. (1988) *J. Am. Chem. Soc.* **110**, 1782.

An, T., Eguchi, T., Akiyama, K. & Hasagawa, Y. (2005) *Appl. Phys. Lett.* **87**, 133114.

Andersen, C.A. & Hinthorne, J.R. (1973) *Anal. Chem.* **45**, 1421.

Annett, J.F. & Haydock, R. (1984) *Phys. Rev. Lett.* **53**, 838.

Annett, J.F. & Haydock, R. (1986) *Phys. Rev. B* **34**, 6860.

Antinodes, E., Janse, E.C. & Sawatzky, G.A. (1977) *Phys. Rev. B* **15**, 1669.

Aono, M., Oshima, C., Zaima, S., Otani, S. & Ishizawa, Y. (1981) *Japan J. Appl. Phys.* **20**, L829.

Aono, M., Katayama, M. & Nomura, E. (1992) *Nucl. Instrum. Methods* **B64**, 29.

Aono, M., Kobayashi, A., Grey, F., Uchida, H. & Huang, D.H. (1993) *Japan J. Appl. Phys.* **32**, 1470.

Armitage, A.F., Woodruff, D.P. & Johnson, P.D. (1980) *Surf. Sci.* **100**, L483.

Ashfold, M.N.R. & Howe, J.D. (1994) *Ann. Rev. Phys. Chem.* **45**, 57.

Auwärter, W., Kreutz, T.J., Greber, T. & Osterwalder, J. (1999) *Surf. Sci.* **429**, 229.

Auwärter, W., Muntwiler, M., Osterwalder, J. & Greber, T. (2003) *Surf. Sci.* **545**, L735.

Bagot, P.A.J., Cerezo, A. & Smith, G.D.W. (2007) *Surf. Sci.* **601**, 2245.

Baikie, I.D. & Estrup, P.J. (1998) *Rev. Sci. Instrum.* **69**, 3902.

Barnes, M.R. & Willis, R.F. (1978) *Phys. Rev. Lett.* **41**, 1729.

Bartels, L., Meyer, G. & Rieder, K.-H. (1997) *Appl. Phys. Lett.* **71**, 213.

Barton, J.J. (1988) *Phys. Rev. Lett.* **61**, 1356.

Barton, J.J. (1991) *Phys. Rev. Lett.* **67**, 3106.

Baumgärtel, P. (2000) Ph.D. thesis, Technical University, Berlin.

Bauer, E. (2012a) *Ultramicrosc.* **119**, 18.

Bauer, E. (2012b) *J. Elect. Spectrosc. Rel. Phenom.* **185**, 314.

Bauer, E., Duden, T. & Zdyb, R. (2002) *J. Phys. D: Appl. Phys.* **35**, 2327.

Beckerle, J.D., Casassa, M.P., Cavanagh, R.R., He Ilweil, E.J. & Stephenson, J.C. (1990) *Phys. Rev. Lett.* **64**, 2090.

Behm, R.J., Christmann, K, Ertl, G & Van Hove, M.A. (1980) *J. Chem. Phys.* **73**, 2984.

Benedek, G., Bernasconi, M., Bohnen, K.-P., Campi, D., Chulkov, E.V., Echenique, P.M., Heid, R., Sklyadneva, I.Y. & Toennies, J.P. (2014) *Phys. Chem. Chem. Phys.* **16**, 7159.

Bergland, C.N. & Spicer, W.E. (1964a) *Phys. Rev.* **136**, A1030.
Bergland, C.N. & Spicer, W.E. (1964b) *Phys. Rev.* **136**, A1044.
Bernardo, D.N., Bhatia, R. & Garrison, B.J. (1994) *Comp. Phys. Commun.* **80**, 259.
Besenbacher, F. (1996) *Rep. Prog. Phys.* **59**, 1737.
Bethe, H. (1928) *Ann. Phys.* **87**, 55.
Beutler, A., Lundgren, E., Nyholm, R., Andersen, J.N., Setlik, B.J. & Heskett, D. (1998) *Surf. Sci.* **396**, 117.
Biberian, J.P. & Van Hove, M.A. (1984) *Surf. Sci.* **138**, 361.
Biesinger, M.C., Lau, L.W.M., Gerson, A.R. & Smart, R.St.C. (2012) *Phys. Chem. Chem. Phys.* **14**, 2434.
Binnig, G., Rohrer, H., Gerber, Ch. & Weibel, E. (1982) *Phys. Rev. Lett.* **49**, 57.
Binnig, G., Quate, C.F. & Gerber, Ch. (1986) *Phys. Rev. Lett.* **56**, 930.
Birgersson, M., Ambladh, C.-O., Morg, M. & Andersen, J.N. (2003) *Phys. Rev. B* **67**, 045402.
Bittencourt, C., Soares, E.A. & Woodruff, D.P. (2003) *Surf. Sci.*, **526**, 33.
Bixler, D.L., Lancaster, J.C., Kontur, F.J., Nordlander, P., Walters, G.K. & Dunning, F.B. (1999) *Phys. Rev. B* **60**, 9082.
Borodin, A. & Reichling, M. (2011) *Phys. Chem. Chem. Phys.* **13**, 15442.
Bradley, M.K., Woodruff, D.P., Robinson, J., Sheppard, D.C. & Hentz, A. (2015) *Surf. Sci.* **635**, 27.
Bradshaw, A.M. & Woodruff, D.P. (2015) *New J. Phys.* **17**, 013033.
Braun, W., Neumann, M., Iwan, M. & Koch, E.E. (1978) *Phys. Stat. Sol. B* **90**, 525.
Braun, W., Steinrück, H.-P. & Held, G. (2005) *Surf. Sci.* **574**, 193.
Brongersma, H.H., Draxler, M., de Ridder, M. & Bauer, P. (2007) *Surf. Sci. Rep.* **62**, 63.
Brown, A. & Vickerman, J.C. (1985) *Surf. Sci.* **151**, 319.
Brown, D., Woodruff, D.P., Noakes, T.C.Q. & Bailey, P. (2001) *Surf. Sci.* **476**, L241.
Brown, D., Quinn, P.D., Woodruff, D.P., Noakes, T.C.Q. & Bailey, P. (2002) *Surf. Sci.* **497**, 1.
Brown, R.D., Hund, Z.M., Campi, D., O'Leary, L.E., Lewis, N.S., Bernasconi, M., Benedek, G. & Sibener, S.J. (2014) *J. Chem. Phys.* **141**, 024702.
Brown, W., Kose, R. & King, D.A. (1998) *Chem. Rev.* **98**, 797.
Brundle, C.R. (1985) *J. Vac. Sci. Technol. A* **3**, 1468.
Brundle, C.R., Behm, R.J. & Barker, J.A. (1984) *J. Vac. Sci. Technol. A* **2**, 1038.
Burema, S.R., Lorente, N. & Bocquet, M.-L. (2012) *J. Chem. Phys.* **136**, 244507.
Bürgi, L., Jeandupeux, O., Hirstein, A., Brune, H. & Kern, K. (1998) *Phys. Rev. Lett.* **81**, 5370.
Bussetti, G., Goletti, C., Chiaradia, P., Rohlfing, M., Betti, M.G., Bussolotti, F., Cirilli, S. *et al.* (2008) *Surf. Sci.* **602**, 1423.
Bussetti, G., Bonanni, B., Cirilli, S., Violante, A., Russo, M., Goletti, C. *et al.* (2011) *Phys. Rev. Lett.* **106**, 067601.
Butz, H.P., Feltgen, R., Pauly, H. & Vehmeyer, H. (1971) *Z. Phys.* **247**, 70.
Cerazo, A., Godfrey, T.J., Sijbrandij, S.J., Smith, G.D.W. & Warren, P.J. (1998) *Rev. Sci. Instrum.* **69**, 49.
Černý, S. (1996) *Surf. Sci. Rep.* **26**, 1.
Chambers, A. (2005) *Modern Vacuum Physics* (Chapman & Hall/CRC, Boca Raton, Fl).
Chambers, A., Fitch, R.K. & Halliday, B.S. (1998) *Basic Vacuum Technology, 2nd edition* (Institute of Physics Publishing, London).
Chambers, S.A. (1991) *Adv. Phys.* **40**, 357.
Chaudhuri, A., Jackson, D.C., Lerotholi, T.J., Jones, R.G., Lee, T.-L., Detlefs, B. *et al.* (2010) *Phys. Chem. Chem. Phys.* **12**, 322.9.

Chen, C.J. (1990) *Phys. Rev. Lett.* **65**, 448.
Chen, C.J. (1992) *Phys. Rev. Lett.* **69**, 1656.
Chen, J.G., Erley, W. & Ibach, H. (1990) *Surf. Sci.* **227**, 79.
Childs, K.D., Carlson, B.A., LaVanier, L.A., Moulder, J.F., Paul, D.F., Stickle, W.F. *et al.* (1995) *Handbook of Auger Electron Spectroscopy, 3rd edition* (Physical Electronics Inc., Chanhassen, Mn, USA).
Childs, T.T., Royer, W.A. & Smith, N.V. (1984) *Rev. Sci. Instrum.* **55**, 1613.
Chiutu, C., Sweetman, A.M., Lakin, A.J., Stannard, A., Jarvis, S., Kantarovich, L. *et al.* (2012) *Phys. Rev. Lett.* **108**, 268302.
Christmann, K., Behm, R.J., Ertl, G., Van Hove, M.A. & Weinberg, W.H. (1979) *J. Chem. Phys.* **70**, 4168.
Chua, F.M., Kuk, Y. & Silverman, P.J. (1989) *Phys. Rev. Lett.* **63**, 386.
Chung, W.F. & Altman, M.S. (1998) *Ultramicrosc.* **74**, 237.
Chung, W.F., Feng, Y.J., Poon, H.C., Chan, C.T., Tong, S.Y. & Altman, M.S. (2003) *Phys. Rev. Lett.* **90**, 216105.
Cinti, R.C. & Nguyen, T.T.A. (1977) *J. Physique* **38**, L29
Claesson, T., Månsson, M., Dallera, C., Venturini, F., De Nadaï, C., Brookes, N.B. *et al.* (2004) *Phys. Rev. Lett.* **93**, 136402.
Cole, R.J., Weightman, P. & Matthew, J.A.D. (2003) *J. Electron Spectrosc. Rel. Phenom.* **133**, 47.
Comsa, G. (1979) *Surf. Sci.* **81**, 57.
Cotte, M., Susini, J., Metrich, N., Moscato, A., Gratzui, C., Bertagnini, A. *et al.* (2006) *Anal. Chem.* **78**, 7484.
Coulman, D.J., Wintterlin, J., Behm. R.J. & Ertl, G. (1990) *Phys. Rev. Lett.* **64**, 1761.
Crapper, M.D., Riley, C.J., Sweeney, P.J.J., McConville, C.F. & Woodruff, D.P. (1987a) *Surf. Sci.* **182**, 213.
Crapper, M.D., Riley, C.E. & Woodruff, D.P. (1987b) *Surf. Sci.* **184**, 121.
Crist, B.V. (2007) *XPS Reports* **1**, 1 (www.xpsdata.com/JAXR_2007/A_Review_of_XPS_Data-banks_BVC.pdf).
Crommie, M.F., Lutz, C.P. & Eigler, D.M. (1993a) *Science* **262**, 218.
Crommie, M.F., Lutz, C.P. & Eigler, D.M. (1993b) *Phys. Rev. B* **48**, 2851.
Crommie, M.F., Lutz, C.P., Eigler, D.M. & Heller, E.J. (1996) *Surf. Sci.* **361**/362, 864.
Crossley, A. & King, D.A. (1977) *Surf. Sci.* **68**, 528.
Crossley, A. & King, D.A. (1980) *Surf. Sci.* **95**, 131.
Crowe, M.C. & Campbell, C.T. (2011) *Ann. Rev. Anal. Chem.* **4**, 41.
Czyzewski, J.J., Madey, T.E. & Yates, J.T., Jr. (1974) *Phys. Rev. Lett.* **32**, 777.
Davenport, J.W. (1976) *Phys. Rev. Lett.* **36**, 945.
Davenport, J.W. (1978) *J. Vac. Sci. Technol.* **15**, 433.
Davila, M.E., Asensio, M.C., Woodruff, D.P., Schindler, K.-M., Hofmann, P., Weiß, K.-U. *et al.* (1994) *Surf. Sci.* **311**, 337.
Davisson, C. & Germer, L.H. (1927) *Phys. Rev.* **30**, 705.
de Crescenzi, M., Diociaiuta, M., Lozzia, L., Picozzia, P., Santucci, S., Battistonib, C. & Mattognob, G. (1986) *Surf. Sci.* **178**, 282.
De Groot, F. & Kotani, A. (2008) *Core Level Spectroscopy of Solids* (CRC Press, Boca Raton, FL).
Delchar, T.A. (1993) *Vacuum Physics and Techniques* (Chapman & Hall, London).
Delchar, T.A. & Tompkins, F.C.C. (1967) *Proc. Roy. Soc. (London)* **A300**, 141.
Delcorte, A. & Garrison, B.J. (2001) *Nucl. Instrum. Methods B* **180**, 37.
Della Pia, A., Riello, M., Floris, A., Stassen, D., Jones, T.S., Bonifazi, D., De Vita, A. & Costantini, G. (2015) *ACS Nano*, in press.

Demuth, J.E. & Eastman, D.E. (1974) *Phys. Rev. Lett.* **32**, 1123.
Denninger, G., Dose, V. & Scheidt, H. (1979) *Appl. Phys.* **18**, 375.
De Jong, A.M. & Niemandsverdriet, J.W. (1990) *Surf. Sci.* **233**, 355.
Djeghloul, F., Ibrahim, F., Cantoni, M., Bowen, M., Joly, L., Boukari, S. *et al.* (2014) *Sci. Rep.* **3**, 1272.
dos Reis, D.D., Negreiros, F.R., de Carvalho, V.E. & Soares, E.A. (2010) *Surf. Sci.* **604**, 568.
Dose, V., Fauster, Th. & Schneider, R. (1986) *Appl. Phys. A* **40**, 203.
Dowsett, M.G. (2003) *Appl. Surf. Sci.* **203**, 5.
Dowsett, M.G. & Barlow, R.D. (1994) *Anal. Chim. Acta* **297**, 253.
Dowsett, M.G., Rowlands, G., Allen, P.N. & Barlow, R.D. (1994) *Surf. Interface. Anal.* **21**, 310.
Draxler, M., Gruber, R., Brongersma, H.H. & Bauer, P. (2002) *Phys. Rev. Lett.* **89**, 263201.
Driver, S.M. & Woodruff, D.P. (2000) *Surf. Sci.* **457**, 11.
Duane, W. & Hunt, F.L. (1915) *Phys. Rev.* **6**, 166.
Duke, P.J. (2008) *Synchrotron Radiation: Production and Properties* (Oxford University Press, Oxford).
Dumpala, S., Broderick, S.R., Bagot, P.A.J. & Rajan, K. (2014) *Ultramicroscopy* **141**, 16.
Duncan, D.A., Unterberger, W., Kreikemeyer-Lorenzo, D. & Woodruff, D.P. (2012a) *Surf. Sci.* **606**, 1298.
Duncan, D.A., Unterberger, W., Jackson, D.C., Knight, M.K., Kröger, E.A., Hogan, K.A. *et al.* (2012b) *Surf. Sci.* **606**, 1435.
Dunning, F.B. & Nordlander, P. (1995) *Nucl. Instrum. Methods B* **100**, 245.
Dutton, G.J. & Robey, S.W. (2013) *J. Phys. Chem. C* **117**, 25414.
Dweydari, A.W. & Mee, C.H.B. (1975) *Phys. Stat. Sol. A* **27**, 223.
Eastman, D.E. & Cashion, J.K. (1971) *Phys. Rev. Lett.* **27**, 1520.
Eastman, D.E., Himpsel, F.J. & van der Veen, J.F. (1982) *J. Vac. Sci. Technol.* **20**, 609.
Echenique, P.M. & Pendry, J.B. (1978) *J. Phys. C* **11**, 2065.
Eigler, D.M. & Schweizer, E.K. (1990) *Nature* **344**, 524.
Einstein, A. (1905) *Ann. Phys. Lpz.* **17**, 132.
Eischens, R.P. & Pliskin, W.A. (1958) *Advan. Catal.* **10**, 1.
Ellis, J., Toennies, J.P. & Witte, G. (1995) *J. Chem. Phys.* **102**, 5059.
Engel, E. & Driezler, R.M. (2011) *Density Functional Theory: An Advanced Course* (Springer, Heidelberg).
Engel, W., Kordesch, M.E., Rotermund, H.H., Kubala, S., & von Oertzen, A. (1991) *Ultramicrosc.* **36**, 148.
Engel-Herbert, R., Schaadt, D.M., Cherifi, S., Bauer, E., Belkhou, R., Locatelli, A. *et al.* (2006) *J. Mag. Mag. Mat.* **305**, 457.
Erlandsson, R., Olsson, L. & Mårtensson, P. (1996) *Phys. Rev. B.* **54**, R8309.
Esbjerg, N. & Nørskov, J.K. (1980) *Phys. Rev. Lett.* **45**, 807.
Estermann, I. & Stern, O. (1930) *Z. Phys.* **61**, 95.
Fauster, T., Weinelt, M. & Höfer, U. (2007) *Prog. Surf. Sci.* **82**, 224.
Feenstra, R., Stroscio, J.A., Tersoff, J. & Fein, A.P. (1987) *Phys. Rev. Lett.* **58**, 1192.
Feibelman, P.J. & McGuire, E.J. (1978) *Phys. Rev. B* **17**, 690.
Feng, R, Liu, A., Liu, S., Shi, J., Zhang, R., & Ren, Z. (2015) *J. Phys. Chem. C* **119**, 9798.
Fiorin, V., Borthwick, D. & King, D.A. (2009) *Surf. Sci.* **603**, 1360.
Fischer-Wolfarth, J.-H., Hartmann, J., Farmer, J.A., Flores-Carmacho, J.M., Campbell, C.T., Schauermann, S. *et al.* (2011) *Rev. Sci. Instrum.* **82**, 024102.
Fisher, A.J. & Blöchl, P.E. (1993) *Phys. Rev. Lett.* **70**, 3263.

Fisher, C.J., Ithin, R., Jones, R.G., Jackson, G.J., Woodruff, D.P. & Cowie, B.C.C. (1998) *J. Phys. Condens. Matter* **10**, L623.
Fishwick, L., Walker, M., Bradley, M.K., Woodruff, D.P. & McConville, D.P. (2012) *Phys. Rev. B* **85**, 045322.
Flege, J.I., Hrbek, J. & Sutter, P. (2008) *Phys. Rev. B* **78**, 165407.
Fleischmann, M., Hendra, P.J. & McQuillan, A.J. (1974) *Chem. Phys. Lett.* **26**, 163.
Fletcher. J.S., Lockyer, N.P. & Vickerman, J.C. (2011) *Mass Spect. Rev.* **30**, 142.
Foley, K.E. & Winograd, N. (1982) *Surf. Sci.* **116**, 1.
Forbes, R.G. (2003) *Ultramicrosc.* **95**, 1.
Fowler, R.H. (1931) *Phys. Rev.* **38**, 45.
Fowler, R.H. & Nordheim, L.W. (1928) *Proc. Roy. Soc.* **A119**, 173.
Franke, K.J., Schulze, G. & Pascual, J.I. (2011) *Science* **332**, 940.
Frenken, J.W.M., Toennies, J.P. & Wöll, Ch. (1988) *Phys. Rev. Lett.* **60**, 1727.
Friedel, J. (1952) *Phil. Mag.* **43**, 153.
Friedel, J. (1958) *Nuovo Cimento* **7**, 287.
Fujikawa, T., Arai, H., Suzuki, R., Shinotsuka, H., Kövér, L. & Ueno, N. (2008) *J. Electron Spectr. Rel. Phenom.* **162**, 146.
Gaarenstroom, S.W. & Winograd, N. (1977) *J. Chem. Phys.* **67**, 3500.
Gadzuk, J.W. (1974a) *Solid State Commun.* **15**, 1011.
Gadzuk, J.W. (1974c) *Phys. Rev. B* **10**, 5030.
Gadzuk, J.W. (1975) *Surf. Sci.* **53**, 132.
Gadzuk, J.W. & Plummer, E.W. (1973) *Rev. Mod. Phys.* **45**, 487.
Gamou, Y., Terai, M., Nagamashima, A. & Oshima, C. (1997) *Sci. Rep. RITU A* **44**, 211.
Garcia, N., Goodman, F.O., Celli, V. & Hill, N.R. (1978) *Phys. Rev. B* **19**, 1808.
Garrison, B.J. (1982) *J. Am. Chem. Soc.* **104**, 6211.
Garrison, B.J., Diebold, A.C., Lin, J.-H. & Sroubek, Z. (1983) *Surf. Sci.* **124**, 461.
Gault, B., Moody, M.P., Cairney, J.M. & Ringer, S.P. (2012) *Atom Probe Microscopy* (Springer).
Giessibl, F.J. (1995) *Science* **267**, 68.
Giessibl, F.J. (1998) *Appl. Phys. Lett.* **73**, 3956 (& Erratum, *ibid.* p. 4070).
Giessibl, F.J. (2003) *Rev. Mod. Phys.* **75**, 949.
Gilmore, C., Marks, L., Grozea, D., Collazo, C., Landree, E. & Twesten, R. (1997) *Surf. Sci.* **381**, 77.
Gladh, J., Öberg, H., Pettersson, L.G.M. & Öström, H. (2015) *Surf. Sci.* **633**, 77.
Glatzel, P., Singh, J., Kvashina, O. & van Bokhoven, J.A. (2010) *J. Am. Chem. Soc.* **132**, 2555.
Glupe, G. & Mehlhorn, W. (1967) *Phys. Lett.* **25A**, 274.
Godfrey, D.J. & Woodruff, D.P. (1980) *J. Phys. E.: Sci. Instrum.* **13**, 969.
Godfrey, D.J. & Woodruff, D.P. (1981) *Surf. Sci.* **105**, 438.
Gomer, R. (1959) *J. Chem. Phys.* **31**, 341.
Grad, G.B., Blaha, P., Schwarz, K., Auwärter, W. & Greber, T. (2003) *Phys. Rev. B* **68**, 085404.
Graham. A.P. (2003) *Surf. Sci. Rep.* **49**, 115.
Gray, A.X., Papp, C., Ueda, S., Balke, B., Yamashita, Y., Plucinski, L., Minár, J. *et al.* (2011) *Nature Mat.* **10**, 759.
Greenler, R.G. (1966) *J. Chem. Phys.* **44**, 310.
Greif, M., Castiglioni, L., Becker-Koch, D., Osterwalder, J. & Hengsberger, M. (2014) *J. Electron. Spectros. Rel. Phenom.* **197**, 30.
Gross, G. & Rieder, K.H. (1991) *Surf. Sci.* **241**, 33.
Gross, G., Müller, V. & Rieder, K.H. (1991) *Phys. Rev. B* **44**, 1434.

Gross, L. (2011) *Nature Chem.* **3**, 273.
Gross, L., Mohn, F., Moll, N., Liljroth, P. & Meyer, G. (2009) *Science* **325**, 1110.
Gross, L., Mohn, F., Moll, N., Meyer, G., Ebel, R., Abdel-Mageed, W.M. *et al.* (2010) *Nature Chem.* **2**, 821.
Gross, L., Moll, N., Mohn, F., Curioni, A., Meyer, G., Hanke, F. *et al.* (2011) *Phys. Rev. Lett.* **107**, 086101.
Gross, L., Mohn, F., Moll, N., Schuler, B., Criado, A., Guitían, E. *et al.* (2012) *Science* **337**, 1326.
Gustafsson, T., Plummer, E.W., Eastman, D.E. & Freeouf, J.L. (1975) *Solid State Commun.* **17**, 391.
Gustafsson, T., Lu, H.C., Busch, B.W., Schulte, W.H. & Garfunkel, E. (2001) *Nucl. Instrum. Methods B* **183**, 146.
Hagstrum, H.D. (1954) *Phys. Rev.* **96**, 336.
Hagstrum, H.D. (1961) *Phys. Rev.* **123**, 758.
Hagstrum, H.D. (1966) *Phys. Rev.* **150**, 495.
Hagstrum, H.D. & Becker, G.E. (1971) *J. Chem. Phys.* **54**, 1015.
Hagstrum, H.D., Petrie, P. & Chaban, E.E. (1988) *Phys. Rev. B* **15**, 10264.
Hamaker, H.C. (1937) *Physica* **4**, 1058.
Hämäläinen, K., Siddons, D.P., Hastings, J.B. & Berman, L.E. (1991) *Phys. Rev. Lett.* **67**, 2850.
Hamers, R.J., Tromp, R.M. & Demuth, J.E. (1986) *Phys. Rev. Lett.* **56**,1972.
Hammaker, R.A., Francis, S.A. & Eischens, R.P. (1965) *Spectrochimica Acta* **21**, 1295.
Hammer, L., Landskon, H., Nichtl-Pecher, W., Fricke, A., Heinz, K. & Müller, K. (1993) *Phys. Rev. B* **47**, 15969.
Hammond, C. & Imam, M.A. (1991) *Ultramicrosc.* **36**, 173.
Hapala, P., Kirchin, G., Wagner, C., Tautz, F.S., Temirov, R. & Jelínek, P. (2014) *Phys. Rev. B* **90**, 085421.
Harada, Y., Masuda, S. & Ozaki, H. (1997) *Chem. Rev.* **97**, 1897.
Harrison, D.E. Jr., Kelly, P.W., Garrison, B.J. & Winograd, N. (1978) *Surf. Sci.* **76**, 311.
Hayden, B.E., Prince, K., Woodruff, D.P. & Bradshaw, A.M. (1983) *Phys. Rev. Lett.* **51**, 475.
Hayward, D.O. & Trapnell, B.M. (1964) *Chemisorption* (Butterworth, London).
Hebenstreit, E.L.D., Hebenstreit, W., Schmid, M. & Varga, P. (1999) *Surf. Sci.* **441**, 441.
Heike, S. & Hashizume, T. (2003) *Appl. Phys. Lett.* **83**, 3620.
Heinrich, A.J., Lutz, C.P., Gupta, J.A. & Eigler, D.M. (2002) *Science* **298**, 1381.
Heinz, K. (1995) *Rep. Prog. Phys.* **58**, 637.
Heinz, K. & Hammer, L. (1996) *Z. Phys. Chem.* **197**, 173.
Heinz, K., Seubert, A. & Saldin, D.K. (2001) *J. Phys.: Condens. Matter* **13**, 10647.
Heinze, S., Blügel, S., Pascal, R., Bode, M. & Wiesendanger, R. (1998) *Phys. Rev. B* **58**, 16432.
Henzler, M. (1977) *Topics in Current Physics*, vol. 4, ed. H. Ibach (Springer-Verlag, Berlin) p. 117.
Henzler, M. (1982) *Appl. Surf. Sci.* **11**/12, 450.
Hessey, S.G. & Jones, R.G. (2015) *Surf. Interface Anal.* **47**, 587.
Hibino, H., Kageshima, H, Maeda, F., Nagase, M., Kobayashi, Y, Kobayashi, Y. & Yamaguchi, H. (2008) *J. Surf. Sci. Nanotechnol.* **6**, 107.
Himpsel, F.J. & Fauster, Th. (1984) *J. Vac. Sci. Technol. A* **2**, 815.
Hla, S.-W., Bartels, L., Meyer, G. & Rieder, K.-H. (2000) *Phys. Rev. Lett.* **85**, 2777.
Ho, W (2002) *J. Chem. Phys.* **117**, 11033.
Hodgson, A. (2000) *Prog. Surf. Sci.* **63**, 1.

Hofer, W.A. (2003) *Prog. Surf. Sci.* **71**, 147.
Hofer, W.A., Garcia-Lekue, A. & Brune, H. (2004) *Chem. Phys. Lett.* **397**, 354.
Höfer, U., Shumay, I.L., Reuss, Ch., Thomann, U., Wallauer, W. & Fauster, Th. (1997) *Science* **277**, 1480.
Hofmann, P. & Schindler, K.M. (1993) *Phys. Rev. B* **47**, 13941.
Hofmann, P., Schindler, K.M., Bao, S., Bradshaw, A.M. & Woodruff, D.P. (1994) *Nature* **368**, 131.
Hofmann, S. (1976) *Appl. Phys.* **9**, 56.
Hofmann, S. (1999) *Surf. Interface Anal.* **27**, 825.
Holland, B.W. & Woodruff, D.P. (1973) *Surf. Sci.* **36**, 488.
Holloway, P.H. & Hudson, J.B. (1974) *Surf. Sci.* **43**, 123.
Holloway, S. & Beeby, J.L. (1978) *J. Phys. C: Solid State Phys.* **11**, L247.
Hu, S.H., Keeffe, M., Yang, Y., Chen, C., Yu, M., Lapeyre, G.J. *et al.* (2000) *Phys. Rev. Lett.* **84**, 939.
Hu, C.-W., Hibino, H., Ogino, T. & Tsong, I.S.T. (2001) *Surf. Sci.* **487**, 191.
Hu, S.H., Wu, H.S., Tong, S.Y., Keeffe, M., Lapeyre, G.J. & Rotenberg, E. (2003) *Surf. Rev. Lett.* **10**, 925.
Huang, D.J., Wu, W.P., Chen, J., Chang, C.F., Chung, S.C., Yuri, M. *et al.* (2002) *Rev. Sci. Instrum.* **73**, 3778.
Hulbert, S.L., Johnson, P.D., Stoffel, N.G., Royer, W.A. & Smith, N.V. (1985) *Phys. Rev. B* **31**, 6815.
Hyde, J.M., Sha, G., Marquis, E.A., Morley, A., Wilford, K.B. & Williams, T.J. (2011) *Ultramicroscopy* **111**, 664.
Ibach, H. (1977b) *Surf. Sci.* **66**, 56.
Ibach, H. (ed.) (1977c) *Topics in Current Physics*, vol. 4 (Springer-Verlag, Berlin) p. 205.
Ibach, H. (1991a) *Electron Energy Loss Spectrometers: The Technology of High Performance*, Springer Series in Optical Sciences, ed. P.W. Hawkes. vol. 63.
Ibach, H. & Mills, D.A. (1982) *Electron Energy Loss Spectroscopy* (Academic Press, London).
Ibanez, J., Garcia, N. & Rojo, J.M. (1983) *Phys. Rev. B* **28**, 3164.
Ichimiya, A. & Cohen, P.I. (2004) *Reflection High-Energy Electron Diffraction* (Cambridge University Press, Cambridge, UK).
Inghram, M.G. & Gomer, R. (1954) *J. Chem. Phys.* **22**, 1279.
International Tables for X-Ray Crystallography (1952) (Kynoch Press, Birmingham, England).
Ishitani, T. & Shimizu, R. (1974) *Phys. Lett.* **46A**, 487.
Jackson, G.J. (1999) Ph.D. thesis, University of Warwick, UK.
Jackson, G.J., Woodruff, D.P., Jones, R.G., Singh, N.K., Chan, A.S.Y., Cowie, B.C.C. *et al.* (2000a) *Phys. Rev. Lett.* **84**, 119.
Jackson, G.J., Cowie, B.C.C., Woodruff, D.P., Jones, R.G., Kariapper, M.S., Fisher, C.J. *et al.* (2000b) *Phys. Rev. Lett.* **84**, 2346.
Jaeger, R., Feldhaus, J., Hasse, J., Stöhr, J., Hussain, Z., Menzel, D. & Norman, D. (1980) *Phys. Rev. Lett.* **45**, 1870.
Jaklevic, R.C. & Lambe, J. (1966) *Phys. Rev. Lett.* **17**, 1139.
James, J. (2007) *Spectrograph Design Fundamentals* (Cambridge University Press, Cambridge, England).
Jensen, F., Besenbacher, F., Lægsgaard, E. & Stensgaard, I. (1990) *Phys. Rev. B* **41**, 10233.
Johansson, B. & Mårtensson, N. (1980) *Phys. Rev. B* **21**, 4427.
Johnson, A.J., Joyce, S.A. & Madey, T.E. (1988) *Phys. Rev. Lett.* **61**, 2578.

Johnson, P.D. (1997) *Rep. Prog. Phys.* **60**, 1217.
Johnson, P.D. & Davenport, J.W. (1985) *Phys. Rev. B* **31**, 7521.
Johnson, P.D. & Güntherodt, G. (2007) in *Handbook of Magnetism and Advanced Magnetic Materials*, ed. H. Kronmuller & S. Parkin (John Wiley & Sons).
Johnson, P.D. & Hulbert, S.L. (1987) *Phys. Rev. B* **35**, 9427.
Johnson, P.D. & Hulbert, S.L. (1990) *Rev. Sci. Instrum.* **61**, 2277.
Johnson, P.D., Hulbert. S.L., Garrett, R.F. & Howells, M.R. (1986) *Rev. Sci. Instrum.* **57**, 1324.
Jones, N., Norris, C., Nicklin, C.L., Steadman, P., Baker, S.H., Johnson, A.D. *et al.* (1998) *Surf. Sci.* **409**, 27.
Jones, R.G. & Woodruff, D.P. (1981) *Vacuum* **31**, 411.
Jones, R.G. & Woodruff, D.P. (1982) *Surf. Sci.* **114**, 38.
Jones, T.S. & Richardson, N.V. (1988) *Phys. Rev. Lett.* **61**, 1753.
Jones, T.S., Ashton, M.R. & Richardson, N.V. (1989) *J. Chem. Phys.* **90**, 7564.
Jones, N., Norris, C., Nicklin, C.L., Steadman, P., Baker, S.H., Johnson, A.D. *et al.* (1998) *Surf. Sci.* **409**, 27.
Jorgensen, W.L. & Salem, L. (1973) *The Organic Chemist's Book of Orbitals* (Academic Press, London).
Kane, E.O. (1964) *Phys. Rev. Lett.* **12**, 97.
Kantrowitz, A. & Grey, J. (1951) *Rev. Sci. Instrum.* **22**, 328.
Katayama, M., Williams, R.S., Kato, M., Nomura, E. & Aono, M. (1991) *Phys. Rev. Lett.* **66**, 2762.
Kawai, M., Komeda, T., Kim, Y., Sainoo, Y. & Katano, S. (2004) *Phil. Trans. Roy. Soc. A* **362**, 1163.
Kawamura, T. & Maksym, P.A. (2014) *Surf. Sci.* **630**, 125.
Kellogg, G.L. (1994) *Surf. Sci. Rep.* **21**, 1.
Kelvin, Lord (1898) *Phil. Mag.* **46**, 82.
Kelvin, Lord (1911) *Mathematical and Physical Papers, vol. IV*, article No. 250 (Cambridge University Press, Cambridge).
Kevan, S.D. (1995) *J. Electron Spectrosc. Rel. Phenom.* **75**, 175.
Kevan, S.D. & Gaylord, R.H. (1987) *Phys. Rev. B* **36**, 5809.
Kevan, S.D., Rosenblatt, D.H., Denley, D.R., Lu, B.-C. & Shirley, D.A. (1978) *Phys. Rev. Lett.* **41**, 1565.
Khatiri, A., Krzyzewski, T.J., McConville, C.F. & Jones, T.S. (2005) *J. Cryst. Growth* **282**, 1.
Kim, Y., Motobayashi, K., Frederiksen, T., Ueba, U. & Kawai, M. (2015) *Prog. Surf. Sci.* **90**, 85.
Kim, Y.D., Wei, T., Wendt, S. & Goodman, D.W. (2003) *Langmuir* **19**, 2929.
King, D.A. (1975) *Surf. Sci.* **47**, 384.
King, D.A. & Thomas, G. (1980) *Surf. Sci.* **92**, 201.
King, D.A. & Wells, M.G. (1972) *Surf. Sci.* **29**, 454.
King, D.A. & Wells, M.G. (1974) *Proc. Roy. Soc. Lond. A* **339**, 245.
King, D.A. & Woodruff, D.P. (ed.) (1982) *The Chemical Physics of Solid Surfaces and Heterogeneous Catalysis, vol. 4, Fundamental Studies of Heterogeneous Catalysis* (Elsevier, Amsterdam).
Kliewer, K.L. (1978) in *Photoemission and the Electronic Properties of Surfaces*, ed. B. Feuerbacher, B. Fitton & R.F. Willis (Wiley, Chichester) p. 45.
Klünker, C., Balden, M., Lehwald, S. & Daum, W. (1996) *Surf. Sci.* **360**, 104.
Knapp, J.A., Himpsel, F.J. & Eastman, D.E. (1979) *Phys. Rev. B* **19**, 4952.
Knotek, M.L. & Feibelman, P.J. (1978) *Phys. Rev. Lett.* **40**, 964.

Knotek, M.L., Jones, V.O. & Rehn, V. (1979) *Phys. Rev. Lett.* **43**, 300.
Kolasinski, K.W. (2012) *Surface Science* (Wiley, New York).
Kolmakov, A., Stultz, J. & Goodman, D.W. (2000) *J. Chem. Phys.* **113**, 7564.
Kono, S., Goldberg, S.M., Hall, N.F.T. & Fadley, C.S. (1978) *Phys. Rev. Lett.* **41**, 1831.
Kontur, F.J., Lancaster, J.C. & Dunning, F.B. (2006) *Surf. Sci.* **600**, 2543.
Koyama, R.Y. & Smith, N.V. (1970) *Phys. Rev. B* **2**, 3049.
Krasovskii, E.E., Höcker, J., Falta, J. & Flege, J.I. (2015) *J. Phys.: Condens. Matter* **27**, 035501.
Krause, M.O. & Ferreira, J.G. (1975) *J. Phys. B* **8**, 2007.
Kreikemeyer-Lorenzo, D., Unterberger, W., Duncan, D.A., Bradley, M.K., Lerotholi, T.J., Robinson, J. *et al.* (2011) *Phys. Rev. Lett.* **107**, 046102.
Kröger, J., Greber, T. & Osterwalder, J. (2000) *Surf. Sci.* **459**, 173.
Kudo, S., Kishimoto, N. & Ohno, K. (2010) *J. Phys. Conf. Series* **235**, 012012.
Kuk, Y., Chua, F.M., Silverman, P.J. & Meyer, J.A. (1990) *Phys. Rev. B* **41**, 12393.
Kukk, E., Ueda, K., Hergenhahn, U., Liu, X.-J., Prümper. G., Yoshida, H. *et al.* (2005) *Phys. Rev. Lett.* **95**, 133001.
Kumpf, C., Marks, L.D., Ellis, D., Smilgies, D., Landemark, E., Nielsen, M. *et al.* (2001) *Phys. Rev. Lett.* **86**, 3586.
Lahee, A.M., Toennies, J.P. & Wöll, Ch. (1987) *Surf. Sci.* **191**, 529.
Lakin, A.J., Chiutu, C., Sweetman, A.M., Moriarty, P. & Dunn, J.L. (2013) *Phys. Rev.B* **88**, 035447.
Landree, E., Marks, L., Zschack, P. & Gilmore, C. (1998) *Surf. Sci.* **408**, 300.
Lang, N.D. (1986a) *Phys. Rev. Lett.* **56**, 1164.
Lang, N.D. (1986b) *Phys. Rev. B.* **34**, 5947.
Lang, N.D. (1987) *Phys. Rev. Lett.* **58**, 45.
Lang, N.D. & Kohn, W. (1970) *Phys. Rev. B* **1**, 4555.
Lang, N.D. & Kohn, W. (1971) *Phys. Rev. B* **3**, 1215.
LaShell, S., McDougall, B.A. & Jensen, E. (1996) *Phys. Rev. Lett.* **77**, 3419.
Lee, J., Fisher, C., Woodruff, D.P., Roper, M.G., Jones, R.G. & Cowie, B.C.C. (2001) *Surf. Sci.* **494**, 166.
Lee, J., Kuzmych, O. & Yates, J.T., Jr. (2005) *Surf. Sci.* **582**, 117.
Lee, P.A. (1976) *Phys. Rev. B* **13**, 5261.
Len, P.M., Zhang, F., Thevuthasan, S., Kaduwela, A.P., Fadley, C.S. & Van Hove, M.A. (1997) *J. Electr. Spectros. Rel. Phenom.* **85**, 145.
Lew, W., Lytken, O., Farmer, J.A., Crowe, M.C. & Campbell, C.T. (2010) *Rev. Sci. Instrum* **81**, 024102.
Liu, Y., Ikeda, D., Nagamatsu, S., Nishi, T., Ueno, N. & Kera, S. (2014) *J. Electron Spectros. Rel. Phenom.* **195**, 287.
Lorente, N. & Persson, M. (2000) *Phys. Rev. Lett.* **85**, 2997.
Lorente, N., Persson, M., Lauhon, L.J., & Ho. W (2001) *Phys. Rev. Lett.* **86**, 2593.
Lu, T.M. & Lagally, M.G. (1980) *Surf. Sci.* **99**, 695.
Lyo, I.W. & Avouris, P. (1991) *Science* **253**, 173.
Lytken O., Lew, W. & Campbell, C.T. (2008) *Chem. Soc. Rev.* **37**, 2172.
Ma, Y., Wassdahl, N., Skytt, P., Guo, J., Nordgren, J., Johnson, P.D. *et al.* (1992) *Phys. Rev. Lett.* **69**, 2598.
Madey, T.E. & Yates, J.T. Jr (1971) *J. Vac. Sci. Technol.* **8**, 525.
Madey, T.E., Yates, J.T. Jr, King, D.A. & Uhlaner, C.J. (1970) *J. Chem. Phys.* **52**, 5215.
Madix, R.J. (1979) *Surf. Sci.* **89**, 540.
Mahapatra, M. & Tysoe, W.T. (2014) *Surf. Sci.* **629**, 132.
Maksym, P.A. (1985) *Surf. Sci.* **149**, 157.

Malterre, D., Kierren, B., Fagot-Revurat, Y., Pons, S., Tejeda, A., Didiot, C. *et al.* (2007) *New J. Phys.* **9**, 391.
Maniraj, M., D'Souza, S.W., Nayak, J., Rai, A., Singh, S., Sekhar, B.N.R. & Barman, S.R. (2011) *Rev. Sci. Instrum.* **82**, 093901.
Manyar, H.G., Morgan, R., Morgan, K., Yang, B., Hu, P., Szlachetko, J., Sá, J. & Hardacre, C. (2013) *Catal. Sci. Technol.* **3**, 1497.
Mapledoram, L.D., Bessent, M.P., Wander, A. & King, D.A. (1994) *Surf. Sci.* **228**, 527.
Margaritondo, G. (1988) *Introduction to Synchrotron Radiation* (Oxford University Press, Oxford).
Marks, L.D. (1999) *Phys. Rev. B* **60**, 2771.
Mårtensson. N., Sokolowski, E. & Svensson, S. (2014) *J. Electron Spectrosc. Rel. Phenom.* **193**, 27.
Martinez, E., Yadav, P., Bouttemy, M., Renault, O., Borowik, Ł., Bertin, F. *et al.* (2013) *J. Electron Spectrosc. Rel. Phenom.* **191**, 86.
Martínez-Galera, A.J., Nicoara, N., Martinez, J.I., Dappe, Y.J., Ortega, J. & Gómez-Rodriguez, J.M. (2014) *J. Phys. Chem. C* **118**, 12782.
Masel, R.I. (1996) *Principles of Adsorption and Reaction on Solid Surfaces* (Wiley-Interscience, New York).
Matsunami, N., Yamamura, Y., Hikawa, Y., Itoh, N., Kazamata, Y., Miyagawa, S. *et al.* (1984) *Atom. Data Nucl. Data Tables* B31B, 1.
Matsushita, T., Agui, A. & Yoshigoe, A. (2005) *J. Electron Spectrosc. Rel. Phenom.*, **144–147**, 1175.
McConville, C.F., Seymour, D.L., Woodruff, D.P. & Bao, S. (1987) *Surf. Sci.* **188**, 1.
McCoy, J.M., Korte, U., Maksym, P.A. & Meyer-Ehmsen, G. (1992) *Surf. Sci.* **261**, 29.
McIntyre, J.D.E. & Aspnes, D.E. (1971) *Surf. Sci.* **24**, 417.
McPhail, D. & Dowsett, M.G. (2009) in *Surface Analysis – The Principal Techniques*, 2nd edition, ed. J. Vickerman & I. Gilmore (Wiley, Chichester) p. 207.
Menteş, T.O. & Locatelli, A. (2012) *J. Electron Spectrosc. Rel. Phenom.* **185**, 323.
Menteş, T.O., Xamborlini, G., Sala, A. & Locatelli, A. (2014) *Belstein J. Nanotechnol.* **5**, 1873.
Menzel, D. & Fuggle, J.C. (1978) *Surf. Sci.* **74**, 321.
Menzel, D. & Gomer, R. (1964) *J. Chem. Phys.* **41**, 3311.
Miller, H.C. (1966) *J. Franklin Inst.* **282**, 382.
Miners, J.H., Gardner, P. & Woodruff, D.P. (2003) *Surf. Sci.* **547**, 355.
Miners, J.H., Gardner, P., Bradshaw, A.M. & Woodruff, D.P. (2004) *J. Phys. Chem. B* **108**, 1708.
Mišković, Z., Vukanic, J. & Madey, T.E. (1984) *Surf. Sci.* **141**, 285.
Mišković, Z., Vukanic, J. & Madey, T.E. (1986) *Surf. Sci.* **169**, 405.
Mochizuki, H., Amana, K., Nojima, M., Oearai, M. & Nihei, Y. (2006) *Surf. Interface Anal.* **38**, 1756.
Moll, N., Gross, L., Mohn, F., Curioni, A., & Meyer, G. (2010) *New. J. Phys.* **12**, 125020.
Moll, N., Schuler, B., Kawai, S., Xu, F., Peng, L., Orita, A. *et al.* (2014) *ACS Nano*, in press.
Moretti, G. (1998) *J. Electron Spectrosc. Rel. Phenom.* **95**, 95.
Morgan, A.E. & Werner, H.W. (1977) *Anal. Chem.* **49**, 927.
Morgenstern, K., Lorente, N. & Rieder, K.-H. (2013) *Phys. Status Solidi B* **250**, 1.
Morgner, H. (2000) *Adv. Atom. Mol. Opt. Phys.* **42**, 387.
Mott, N.F. (1929) *Proc. Roy. Soc. A* **124**, 425.
Mott, N.F. (1932) *Proc. Roy. Soc. A* **135**, 429.
Müller, E.W. (1936) *Z. Phys.* **37**, 838.

Müller, E.W. (1951) *Z. Phys.* **131**, 136.
Müller, E.W. (1956) *Phys. Rev.* **102**, 618.
Muñoz-Márquez, M.A., Tanner, R.E. & Woodruff, D.P. (2004) *Surf. Sci.* **565**, 1.
Nabhan, W., Equer, B., Broniatowski, A. & De Rosny, G. (1997) *Rev. Sci. Instrum.* **68**, 3108.
Neddermeyer, H. & Drechsler, M. (1988) *J. Microscopy* **152**, 459.
Niehus, H., Heiland, W. & Taglauer, E. (1993) *Surf. Sci. Rep.* **17**, 213.
Nilsson, A., Weinelt, M., Wiell, T., Bennich, P., Karis, O., Wassdahl, N. *et al.* (1997) *Phys. Rev. Lett.* **78**, 2847.
Nilsson, A. & Pettersson, L.G.M. (2004) *Surf. Sci. Rep.* **55**, 49.
Nilsson, V., Van den Bossche, M., Hellman, A. & Grönbeck, H. (2015) *Surf. Sci.* **640**, 59.
Nonnenmacher, M., O'Boyle, M.P. & Wickramasinghe, H.K. (1991) *Appl. Phys. Lett.* **58**, 2921.
Nordgren, J. & Rubensson, J.-E. (2013) *J. Electron Spectrosc. Rel. Phenom.* **188**, 3.
Nordheim, L.W. (1928) *Proc. Roy. Soc. A* **121**, 626.
Norman, D. & Woodruff, D.P. (1979) *Surf. Sci.* **79**, 76.
NPL (2005) www.npl.co.uk/science-technology/surface-and-nanoanalysis/services/sputter-yield-values
O'Connor, D.J. & Biersack, J.P. (1985) *Bucl. Instrum. Methods B* **15**, 14.
Oechsner, H. (1973) *Z. Phys.* **261**, 37.
Oen, O.S. (1983) *Surf. Sci.* **131**, L407.
Offenbacher, H., Lüftner, D., Ules, T., Reinisch, E.M., Koller, G., Puschnig, P. *et al.* (2015) *J. Electron Spectrosc. Rel. Phenom.* **204, Part A**, 92–101.
Ogorodnikov, I.I., Vorokh, A.S., Titov, A.N. & Kuznetsov, M.V. (2012) *JETP Lett.* **95**, 372.
Orders, P.J., Kono, S., Fadley, C.S. Trehan, R. & Lloyd, J.T. (1982) *Surf. Sci.* **119**, 371.
Ossowski, J., Rysz, J., Krawiec, M., Maciazek, D., Postwana, Z., Terfort, A. *et al.* (2015) *Angew. Chem. Int. Ed.* **54**, 1336.
Osterwalder, J (2006) in *Magnetism: A Synchrotron Radiation Approach*, ed. E. Beaurepaire, H. Bulou, F. Scheurer & J.-P. Kappler, *Lecture Notes in Physics*, vol. 697 (Springer, Berlin), p. 95.
Paavilainen, S. & Persson, M. (2006) *Phys. Rev. B.* **74**, 085417.
Palermo, V., Palma, M. & Samori, P. (2006) *Adv. Mater.* **18**, 145.
Palmer, R.E. & Rous, P.J. (1992) *Rev. Mod. Phys.* **64**, 383.
Palotás, K., Mándi, G. & Szunyogh, L. (2012) *Phys. Rev. B.* **86**, 235415.
Park, R.L., Houston, J.E. & Schreiner, D.G. (1971) *Rev. Sci. Instrum.* **42**, 60.
Park, R.L. & Madden, H.H. Jr (1968) *Surf. Sci.* **11**, 188.
Pascal, M., Lamont, C.L.A., Kittell, M., Hoeft, J.T., Terborg, R., Polcik, M. *et al.* (2001) *Surf. Sci.* **492**, 285.
Pavliček, N., Herranz-Lancho, C., Fleury, B., Neu, M., Niedenführ, J., Ruben, M. *et al.* (2013) *Phys. Status Solidi B* **250**, 2424.
Pendry, J.B. (1974) *Low Energy Electron Diffraction* (Academic Press, London).
Pendry, J.B. (1980) *J. Phys. C–Solid State Phys.* **13**, 937.
Pendry, J.B. (1981) *J. Phys. C* **14**, 1381.
Pendry, J.B. & Saldin, D.K. (1984) *Surf. Sci.* **145**, 33.
Perdereau, J. & Rhead, G.E. (1971) *Surf. Sci.* **24**, 555.
Persson, B.N.J., Hoffmann, F.M. & Ryberg, R. (1986) *Phys. Rev. B* **34**, 2266.
Pessa, M., Lindroos, M., Asonem, H. & Smith, N.V. (1982) *Phys. Rev. B* **25**, 738.
Petersen, L., Sprunger, P.T., Hofmann, P., Lægsgaard, E., Brinner, B.G., Doering, M. *et al.* (1998) *Phys. Rev. B.* **57**, R6859.

Petersson, L.-G., Kono, S., Hall, N.F.T., Fadley, C.S. & Pendry, J.B. (1979) *Phys. Rev. Lett.* **42**, 1545.
Plummer, E.W., Tonner, B., Holzwarth, N. & Liebsch, A. (1980) *Phys. Rev. B* **21**, 4306.
Poelsma, B., de Zwart, S.T. & Comsa, G. (1983) *Phys. Rev. Lett.* **51**, 522.
Postawa, Z., Czerwinski, B., Szewczyk, M., Smiley, E.J., Winograd, N. & Garisson, B.J. (2004) *J. Phys. Chem. B* **108**, 7831.
Primetzhofer, D., Markin, S.N., Juaristi, J.I., Taglauer, E. and Bauer, P. (2008) *Phys. Rev. Lett.* **100**, 213201.
Prutton, M. & El Gomati, M. (ed.) (2006) *Scanning Auger Electron Microscopy* (John Wiley & Sons).
Puschmann, A., Haase, J., Crapper, M.D., Riley, C.E. & Woodruff, D.P. (1985) *Phys. Rev. Lett.* **54**, 2250.
Puschnig, P., Berkebile, S., Fleming, A.J., Koller, G., Emtsev, K., Seyller, T. *et al.* (2009) *Science* **326**, 702.
Quinn, J.J. (1962) *Phys. Rev.* **126**, 1453.
Ramsier, R.D. & Yates, J.T., Jr. (1991) *Surf. Sci. Rep.* **12**, 243.
Redhead, P.A. (1962) *Vacuum* **12**, 203.
Redhead, P.A. (1964) *Can. J. Phys.* **42**, 886.
Reimann, C.T., El-Maazawi, M., Walzi, K., Garrison, B.J., Winograd, N. & Redhead, P.A. (1967) *Nuovo Cimento Suppl.* **5**, 586.
Reid, R.J. (1972) *Surf. Sci.* **29**, 623.
Richardson, N.V. (1983) *Chem. Phys. Lett.* **102**, 390.
Reuter, K., Schadt, J., Bernhardt, J., Wedler, K., Starke, U. & Heinz, K. (1998) *Phys. Rev. B* **58**, 10806.
Robinson, I.K. (1986) *Phys. Rev. B* **33**, 3830.
Robinson, N.W. (1968) *The Physical Principles of Ultra-High Vacuum Systems and Equipment* (Chapman & Hall, London).
Rotermund, H.H. (1993) *Surf. Sci.* **283**, 87.
Rousseau, P., Khemliche, H., Borisov, A.G. & Roncin, P. (2007) *Phys. Rev. Lett.* **98**, 016104.
Roy, D. & Carette, J.D. (1977) in *Topics in Current Physics*, vol. 4, ed. H. Ibach (Springer-Verlag, Berlin).
Ruan, L., Besenbacher, F., Stensgaard, I. & Lægsgaard, E. (1993) *Phys. Rev. Lett.* **70**, 4079.
Rupprechter, G., Dellwig, T., Unterhalt, H. & Freund, H.-J. (2001) *Top. Catal.* **15**, 19.
Sacks, W. (2000) *Phys. Rev. B* **61**, 7656.
Safonova, O.V., Tromp, M., van Bokhoven, J.A., de Groot, F.M.F., Evans, J. & Glatzel, P. (2006) *J. Phys. Chem. B* **110**, 16162.
Saiki, R.S., Kaduwela, A.P., Kim, Y.J., Friedman, D.J., Osterwalder, J., Thevuthasan, S. *et al.* (1992) *Surf. Sci.* **279**, 305.
Saldin, D.K. (1997) *Surf. Rev. Lett.* **4**, 441.
Sautet, P. (1997a) *Surf. Sci.* **374**, 406.
Sautet, P. (1997b) *Chem. Rev.* **97**, 1097.
Sawatzky, G.A. & Lenselink, A. (1980) *Phys. Rev. B* **21**, 1790.
Schedin, F., Warburton, R. & Thornton, G. (1998) *Rev. Sci. Instrum.* **69**, 2297.
Schindler, K.-M., Hofmann, P., Weiß, K.-U., Dippel, R., Gardner, P., Fritzsche, V. & González-Elipe, A.R. (1993) *J. Electron Spectrosc. Rel. Phenom.* **64/65**, 75.
Schmid, M., Stadler, H. & Varga, P. (1993) *Phys. Rev. Lett.* **70**, 1441.
Schüller, A. & Winter, H. (2009) *Nucl. Instrum. Methods B* **267**, 628.
Schüller, A., Wethekam, S. & Winter, H. (2007) *Phys. Rev. Lett.* **98**, 016103.

Schweitzer, E., Persson, B.N.J., Tüshaus, M., Hodge, D. & Bradshaw, A.M. (1989) *Surf. Sci.* **213**, 49.
Seah, M.P. (2005) *Nucl. Instrum. Methods B* **229**, 348.
Seah, M.P. & Dench, W.A. (1979) *Surf. Interface Analysis* **1**, 2.
Seah, M.P., Clifford, C.A., Green, F.M. & Gilmore, I.S. (2005) *Surf. Interface Anal.* **37**, 444.
Sekiyama, A., Higashiya, A. & Imada, S. (2013) *J. Electron Spectrosc. Rel. Phenom.* **190**, 201.
Seo, Y. & Jhe, W. (2008) *Rep. Prog. Phys.* **71**, 016101.
Sevier, K.D. (1972) *Low Energy Electron Spectrometry* (Wiley, New York).
Sheppard, N. & Nguyen, N.T. (1978) *Adv. IR Raman Spect.* **5**, 67.
Shevchik, N.J. (1977) *J. Phys. C* **10**, L555.
Shirasawa, T., Voegeli, W., Nojima, T., Iwasawa, Y., Yamaguchi, Y. & Takahashi, T. (2014) *Phys. Rev. Lett.* **113**, 165501.
Shirley, D.A. (1973) *Advan. Chem. Phys.* **23**, 85.
Sholl, D. & Steckel, J.A. (2009) *Density Functional Theory* (Wiley, Hoboken, New Jersey).
Sigmund, P. (1969) *Phys. Rev.* **184**, 383.
Smith, N.V. (1988) *Rep. Prog. Phys.* **51**, 1227.
Smith, N.V.& Woodruff, D.P. (1987) *Prog. Surf. Sci.* **21**, 295.
Smith, R.J., Anderson, J. & Lapeyre, G.J. (1976) *Phys. Rev. Lett.* **37**, 1081.
Smith, N.V., Benbow, R.L. & Hurych, Z. (1980) *Phys. Rev. B* **21**, 4331.
Smoluchowski, R. (1941) *Phys. Rev.* **60**, 661.
Soares, E.A., de Castillho, C.M.C. & de Carvalho, V.E. (2011) *J Phys.: Condens. Matter* **23**, 303001.
Souda, R. & Aono, M. (1986) *Nucl. Instrum. Methods B* **15**, 114.
Spitzl, R., Niehus, H. & Comsa, G. (1990) *Rev. Sci. Instrum.* **61**, 760.
Steinmann, W. (1989) *Appl. Phys. A.* **49**, 365.
Stiles, P.L., Dieringer, J.A., Shah, N.C. & Van Duyne, R.P. (2008) *Ann. Rev. Anal. Chem.* **1**, 601.
Stipe, B.C., Rezaei, M.A. & Ho, W. (1998) *Science* **280**, 1732.
Stipe, B.C., Rezaei, M.A. & Ho, W. (1999) *Phys. Rev. Lett.* **82**, 1724.
Stobie, R.W., Rao, B. & Dignam, M.J. (1976) *Surf. Sci.* **56**, 334.
Stöhr, J. & Jaeger, R. (1982) *Phys. Rev. B.* **26**, 4111.
Stöhr, J. (1992) *NEXAFS Spectroscopy: Springer Series in Surface Science,* vol. 25 (Springer, Berlin).
Stroscio, J.A. & Eigler, D.M. (1991) *Science* **254**, 1319.
Stroscio, J.A., Feenstra, R.M. & Fein, A.P. (1986) *Phys. Rev. Lett.* **57**, 2579.
Suga, S., Sekiyama, A., Fujiwara, H., Nakatsu, Y., Miyamachi, T., Imada, S., Baltzer, P. *et al.* (2009) *New. J. Phys.* **11**, 073025.
Suga, S., Itoda, S., Sekiyama, A., Fujiwara, H., Komori, S., Imada, S. *et al.* (2012) *Phys. Rev. B.* **86**, 035146.
Sun, J., Hannon, J.B., Kellogg, G.L. & Pohl, K. (2007) *Phys. Rev. B* **76**, 205414.
Sun, J., Hannon, J.B., Tromp, R.M., Johari, P., Bol, A.A., Shenoy, V.B. *et al.* (2010) *ACS Nano* **4**, 7073.
Surnev, L., Xu., Z. & Yates, J.T. Jr. (1988) *Surf. Sci.* **201**, 1.
Sutcu, L.F., White, H.W. & Wragg, J.L. (1991) *Surf. Sci.* **249**, L343.
Suzuki, T.T., Kuwahara, H. & Yamauchi, Y. (2010) *Surf. Sci.* **604**, 1767.
Sweetman, A., Rahe, P. & Moriarty, P. (2014a) *Nano Lett.* **14**, 2265.
Sweetman, A.M., Jarvis, S.P., Sang, H., Lekkas, I., Rahe, P., Wang, Y. *et al.* (2014b) *Nature Commun.* **5**, 3931.

Taglauer, E. & Heiland, W. (1976) *Appl. Phys.* **9**, 261.
Taglauer, E., Englert, W., Heiland, W. & Jackson, D.P. (1980) *Phys. Rev. Lett.* **45**, 740.
Takahashi, T., Sumitani, K. & Kusano, S. (2001) *Surf. Sci.* **493**, 36.
Takayanagi, K., Tanishiro, Y., Takahashi, M. & Takahashi, S. (1985a) *J. Vac. Sci. Technol. A.* **3**, 1502.
Takayanagi, K., Tanishiro, Y., Takahashi, M. & Takahashi, S. (1985b) *Surf. Sci.* **164**, 367.
Taylor, J.L. & Weinberg, W.H. (1978) *J. Vac. Sci. Technol.* **15**, 1811.
Taylor, R.S. & Garrison, B.J. (1994a) *J. Am. Chem. Soc.* **116**, 4465.
Taylor, R.S. & Garrison, B.J. (1994b) *Chem. Phys. Lett.* **230**, 495.
Telieps, W. & Bauer, E. (1985) *Ultramicrosc.* **17**, 57.
Terborg, R., Baumgärtel, P., Lindsay, R., Schaff, O., Gießel, T., Hoeft, J.T. *et al.* (2000) *Phys. Rev. B* **61**, 16697.
Terborg, R., Polcik, M., Hoeft, J.T., Kittel, M., Sayago, D.I., Toomes, R.L. *et al.* (2002) *Phys. Rev. B* **66**, 085333.
Tersoff, J. & Hamann, D.R., (1983) *Phys. Rev. Lett.* **50**,1998.
Tersoff, J. & Hamann, D.R., (1985) *Phys. Rev. B* **31**, 2.
Tersoff, J., Jesson, D.E. & Tang, W.X. (2009) *Science* **324**, 236.
Tong, S.Y., Li., C.H. & Mills, D.L. (1980) *Phys. Rev. Lett.* **44**, 407.
Tong, S.Y., Li., C.H. & Mills, D.L. (1981) *Phys. Rev. Lett.* **24**, 806.
Toomes, R.L., Woodruff, D.P., Polcik, M., Bao, S., Hofmann, P., Schindler, K.M. *et al.* (2000) *Surf. Sci.* **445**, 300.
Torbrügge, S., Schaff, O. & Rychen, J. (2010) *J. Vac. Sci. Technol. B* **28**, C4E12.
Tracy, J.C. & Palmberg, P.W. (1969) *Surf. Sci.* **14**, 274.
Traum, M.M. & Woodruff, D.P. (1980) *J. Vac. Sci. Technol.* **17**, 1202.
Trigwell, S. (1993) *VG Scientific Auger Handbook* (VG Scientific, East Grinstead, UK).
Troisi, A. & Ratner, M.A. (2006) *J. Chem. Phys.* **125**, 214709.
Tromp, R.M. (2000) *IBM J. Res, Develop.* **44**, 503.
Tromp, R.M. (2012) *Ultramicrosc.* **120**, 73.
Tromp, R.M. & van der Veen, J.F. (1983) *Surf. Sci.* **133**, 159.
Tromp, R.M., Hamers, R.J. & Demuth, J.E. (1986a) *Phys. Rev. B* **34**, 1388.
Tromp, R.M., Hamers, R.J. & Demuth, J.E. (1986b) *Science* **234**, 304.
Tromp, R.M., Mankos, M., Reuter, M.C., Ellis, A.W. & Copel, M. (1998) *Surf. Rev. Lett.* **5**, 1189.
Tromp, R.M., Hannon, J.B., Ellis, A.W., Wan, W., Berghaus, A. & Schaff, O. (2010) *Ultramicrosc.* **110**, 852.
Troyan, V.I., Borisyuk, P.V., Kashurnikov, V.A., Krasavin, A.V., Borman, V.D. & Tronin, V.I. (2013) *Phys. Lett. A* **377**, 405.
Tsong, T.T. (1971) *J. Chem. Phys.* **54**, 4205.
Tsong, T.T. (1993) *Surf. Sci.* **299/300**, 153.
Tsukada, M., Kobayashi, K. & Isshiki, N. (1993) *Appl. Surf. Sci.* **67**, 235.
Tully, J.C., (1977) *Phys. Rev. B* **16**, 4324.
Turner, D.W., Baker, C., Baker, A.D. & Brundle, C.R., (1970) *Molecular Photoelectron Spectroscopy* (InterSci., New York).
Uchida, H., Huang, D., Grey, F. & Aono, M. (1993) *Phys. Rev. Lett.* **70**, 2040.
Valla, T., Johnson, P.D., Dhesi, S.S., Smith, K.E., Doppalapudi, D., Moustakas, T.D. *et al.* (1999) *Phys. Rev. B* **59**, 5003.
van den Berg, J.A., Reading, M.A., Bailey, P., Noakes, T.Q.C., Adelmann, C., Popovic, M. *et al.* (2013) *Appl. Surf. Sci.* **281**, 8.
van der Veen, J.F. (1985) *Surf. Sci. Reports* **5**, 199.
Vandervorst, W. (2008) *Appl. Surf. Sci.* **255**, 805.

Van Hove, J.M., Pukite, P., Cohen, P.I. & Lent, C.S. (1983) *J. Vac. Sci. Technol. A*, **1**, 609.
Van Hove, M.A., Weinberg, W.H. & Chan, C.-M. (2011) *Low Energy Electron Diffraction, Experiment, Theory and Surface Structure Determination* (Springer-Verlag, Berlin). Paperback reprint of the original 1986 publication.
Vickerman, J.C., Oakes, A. & Gamble, H. (2000) *Surf. Interface. Anal.* **29**, 349.
Victoreen, J.A. (1943) *J. Appl. Phys.* **14**, 95.
Vitali, L., Levita, G., Ohmann, R., Comisso, A., De Vita, A. & Kern, K. (2010) *Nature Materials* **9**, 320.
Voegeli, W., Aoyama, T., Akimoto, K., Ichimiya, A., Hisada, Y., Mitsuoka, Y. & Mukainakano, S. (2010) *Surf. Sci.* **604**, 1713.
Von Oertzen, A., Rotermund, H.H. & Nettesheim, S. (1994) *Surf. Sci.* **311**, 322.
Vorburger, T.V., Penn, D. & Plummer, E.W. (1975) *Surf. Sci.* **48**, 417.
Wagner, C.D. (1975) *Faraday Disc. Chem. Soc.* **60**, 291.
Wagner, C.D., Riggs, W.M., Davis, L.E., & Moulder, J.F. (1979) *Handbook of X-ray Photoelectron Spectroscopy*, ed. G. Muilenberg (Perkin-Elmer, MN, USA).
Wagner, T., Wang, J.Y. & Hofmann, S. (2003) in *Surface Analysis by Auger Electron Spectroscopy and X-ray Photoelectron Spectroscopy*, ed. D. Briggs & J.T. Grant (IM Publications, Chichester, UK) p. 619.
Walker, M., Parkinson, C.R., Draxler, M. & McConville, C.F. (2005) *Surf. Sci.* **584**, 153.
Walker, M, Brown, M.G., Draxler, M., Fishwick, L., Dowsett, M.G. & McConville, C.F. (2011) *Surf. Sci.* **605**, 107.
Walmsley, D.G. & Tomlin, J.L. (1985) *Prog. Surf. Sci.* **18**, 247.
Wang, G.C. & Lagally, M.G. (1979) *Surf. Sci.* **81**, 69.
Wang, N.P., García, E.A., Flores, F., Goldberg, E.C., Brongersma, H.H. & Bauer, P. (2001) *Phys. Rev. A* **64**, 012901.
Watson, P.R., Van Hove, M.A. & Hermann, K. (2003) *NIST Surf. Structure Database Ver. 5.0*, NIST Gaithersburg, MD.
Weinelt, M. (2002) *J. Phys. Condens. Matter* **14**, R1099.
Wellendorf, J., Silbaugh, T.L., Garcia-Pintos, D., Nørskov, J.K., Bligaard, T., Stidt, F. *et al.* (2015) *Surf. Sci.* **640**, 36.
Williams, A.R. & Lang, N.D. (1977) *Surf. Sci.* **68**, 138.
Williams, G.P. (1986) Section 1.1 of X-ray Data Booklet, Lawrence Berkeley Laboratory, http://xdb.lbl.gov/Section1/Sec_1-1.html
Williams, P. (1979) *Surf. Sci.* **90**, 588.
Williams, R.P., Nicklin, C.L., Alcock, S.G., Howes, P.B. & Bennett, S.L. (2015) to be published.
Willmott, P.R. (2011) *An Introduction to Synchrotron Radiation: Techniques and Applications* (John Wiley, Chichester).
Window, A.J., Hentz, A., Sheppard, D.C., Parkinson, G.S., Woodruff, D.P., Unterberger, W. *et al.* (2012) *Surf. Sci.* **606**, 1716.
Winograd, N. (2013) *Surf. Interface Anal.* **45**, 3.
Winter, H. & Schüller, A. (2011) *Prog. Surf. Sci.* **86**, 169.
Wintterlin, J., Wiechers, J., Burne, H., Gritsch, T., Höfer, H. & Behm, R.J. (1989) *Phys. Rev. Lett.* **62**, 59.
Wittmaack, K. (2013) *Surf. Sci. Rep.* **68**, 108.
Wolf, M., Knoesel, E. & Hertel, T. (1996) *Phys. Rev. B.* **54**, R5295.
Wood, E.A. (1964) *J. Appl. Phys.* **35**, 1306.
Woodruff, D.P. (2007) *Surf. Sci. Rep.* **62**, 1.
Woodruff, D.P. & Bradshaw, A.M. (1994) *Rep. Prog. Phys.* **57**, 1029.

Woodruff, D.P., Norman, D., Holland, B.W., Smith, N.V., Farrell, H.H. & Traum, M.M. (1978) *Phys. Rev. Lett.* **41**, 1130.
Woodruff, D.P., Johnson, P.D., Traum, M.M., Farrell, H.H., Smith, N.V., Benbow, R.L. *et al.* (1981) *Surf. Sci.* **104**, 282.
Woodruff, D.P., Johnson, P.D. & Smith, N.V. (1983) *J. Vac. Sci. Technol. A* **1**, 1104.
Woodruff, D.P., Seymour, D.L., McConville, C.F., Riley, C.E., Crapper, M.D., Prince, N.P. *et al.* (1988a) *Surf. Sci.* **195**, 237.
Woodruff, D.P., McConville, C.F., Kilcoyne, A.L.D., Lindner, T., Somers, J., Surman, M., Paolucci. G. & Bradshaw, A.M. (1988b) *Surf. Sci.* **201**, 228.
Woodruff, D.P., Baumgärtel, P., Hoeft, J.T., Kittel, M. & Polcik, M. (2001) *J. Phys.: Condens. Matter* **13**, 10625.
Wu, H., Lapeyre, G.J., Huang, H. & Tong, S.Y. (1993) *Phys. Rev. Lett.* **71**, 251.
Yamauchi, Y. & Kurahashi, M. (2001) *Appl. Surf. Sci.* **169–170**, 236.
Yates, J.T., Jr. (2012) *J. Chem. Phys.* **137**, 091701.
Yates, J.T. Jr. & Madey, T.E. (1971b) *J. Vac. Sci. Technol.* **8**, 63.
Yeh, J.J. & Lindau, I. (1985) *At. Data Nucl. Data Tables* **32**, 1.
Yin, L., Tsang, T. & Adler, I. (1976) *J. Elect. Spect.* **9**, 67.
Zanazzi, E. & Jona, F. (1977) *Surf. Sci.* **62**, 61.
Zegenhagen, J. & Kazimirov, A. (ed.) (2013) *The X-ray Standing Wave Technique: Principles and Applications* (World Scientific, Singapore).
Zharnikov, M., Weinelt, M., Zebisch, P., Stichler, M. & Steinrück, H.P. (1994) *Phys. Rev. Lett.* **73**, 3548.
Ziegler, J.F. (2004) *Nucl. Instrum. Methods B*, **219–220**, 1027. The SRIM software package can be downloaded from www.SRIM.org.
Ziegler, J.F., Biersack, J.P. & Littmark, U. (1985) *The Stopping and Range of Ions in Solids* (Pergamon, New York).
Zisman, W.A. (1932) *Rev. Sci. Instrum.* **3**, 367.
Zhang, J., Chen, P., Yuan, B., Ji, W., Cheng, Z. & Qui, X. (2013) *Science* **342**, 611.
Zhou, C., Ma, Z., Ren, Z., Wodtke, A.M. & Yang, X. (2012) *Energy Envir. Sci.* **5**, 6833.