Bibliography

[1] R.P. Feynman.
There's Plenty of Room at the Bottom, February 1960.
http://www.zyvex.com/nanotech/feynman.html.

[2] A. Aviram and M.A. Ratner.
Molecular rectifiers.
Chemical Physics Letters, 29(2):277–283, 1974.

[3] S.R. Forrest.
Ultrathin Organic Films Grown by Organic Molecular Beam Deposition and Related Techniques.
Chemical Review, 97:1793, 1997.

[4] J.H. Burroughes, D.D.C. Bradley, A.R. Brown, R.N. Marks, K. Mackay, R.H. Friend, P.L. Burns, and A.B. Holmes.
Light-emitting diodes based on conjugated polymers.
Nature, 347(6293):539–541, 1990.

[5] J. Liu, L.N. Lewis, and A.R. Duggal.
Photoactivated and patternable charge transport materials and their use in organic light-emitting devices.
Applied Physics Letters, 90:233503, 2007.

[6] M. Granstrom, K. Petritsch, A.C. Arias, A. Lux, M.R. Andersson, and R.H. Friend.
Laminated fabrication of polymeric photovoltaic diodes.
Nature, 395(6699):257–260, 1998.

[7] P. Peumans and S.R. Forrest.
Very-high-efficiency double-heterostructure copper phthalocyanine/C_{60} photovoltaic cells.
Applied Physics Letters, 79(1):126–128, 2001.

[8] P. Peumans, S. Uchida, and S.R. Forrest.
Efficient bulk heterojunction photovoltaic cells using small-molecular-weight organic thin films.
Nature, 425(6954):158–162, 2003.

[9] Max S., Jonathan M., Jay B.B., and Stephen R.F.
Effects of film morphology and gate dielectric surface preparation on the electrical characteristics of organic-vapor-phase-deposited pentacene thin-film transistors.

Applied Physics Letters, 81(2):268–270, 2002.

[10] D.V. Konarev, N.V. Drichko, R.N. Lyubovskaya, Y.M. Shul'ga, A.L. Litvinov, V.N. Semkin, Y.A. Dubitsky, and A. Zaopo.
Donor–acceptor interaction of fullerene C_{60} with triptycene in molecular complex TPC·C_{60}.
Journal of Molecular Structure, 526(1-3):25–29, 2000.

[11] E.M. Veen, B.L. Feringa, P.M. Postma, H.T. Jonkman, and A.L. Spek.
Solid state organisation of C_{60} by inclusion crystallisation with triptycenes.
Chemical Communications, 1999(17):1709–1710, 1999.

[12] W. Ho.
Single-molecule chemistry.
The Journal of Chemical Physics, 117:11033, 2002.

[13] G. Binnig, H. Rohrer, C. Gerber, and E. Weibel.
Tunneling through a controllable vacuum gap.
Applied Physics Letters, 40:178, 1982.

[14] G. Binnig, H. Rohrer, Ch. Gerber, and E. Weibel.
Surface Studies by Scanning Tunneling Microscopy.
Physical Review Letters, 49(1):57–61, Jul 1982.

[15] G. Binnig, H. Rohrer, Ch. Gerber, and E. Weibel.
7×7 Reconstruction on Si(111) Resolved in Real Space.
Physical Review Letters, 50(2):120–123, Jan 1983.

[16] J. Tersoff and D.R. Hamann.
Theory and Application for the Scanning Tunneling Microscope.
Physical Review Letters, 50(25):1998–2001, Jun 1983.

[17] J. Bardeen.
Tunnelling from a Many-Particle Point of View.
Physical Review Letters, 6(2):57–59, January 1961.

[18] N.D. Lang.
Spectroscopy of single atoms in the scanning tunneling microscope.
Physical Review B, 34(8):5947–5950, Oct 1986.

[19] A. Selloni, P. Carnevali, E. Tosatti, and C.D. Chen.
Voltage-dependent scanning-tunneling microscopy of a crystal surface: Graphite.
Physical Review B, 31(4):2602–2605, Feb 1985.

[20] A. Sinsarp, Y. Yamada, M. Sasaki, and S. Yamamoto.
Microscopic Study on the Work Function Reduction Induced by Cs-Adsorption.
Japanese journal of Applied Physics, 42:4882–4886, 2003.

[21] J.I. Pascual, C. Corriol, G. Ceballos, I. Aldazabal, H.P. Rust, K. Horn, J.M. Pitarke, P.M. Echenique, and A. Arnau.
Role of the electric field in surface electron dynamics above the vacuum level.
Physical Review B, 75(16):165326, 2007.

[22] K. Burke.
The ABC of DFT, April 2003.

URL: *http://dft.rutgers.edu/kieron/beta*.

[23] P. Hohenberg and W. Kohn.
Inhomogeneous Electron Gas.
Physical Review, 136(3B):B864–B871, Nov 1964.

[24] W. Kohn and L.J. Sham.
Self-Consistent Equations Including Exchange and Correlation Effects.
Physical Review, 140(4A):A1133–A1138, Nov 1965.

[25] M.C. Payne, M.P. Teter, D.C. Allan, T.A. Arias, and J.D. Joannopoulos.
Iterative minimization techniques for ab initio total-energy calculations: molecular dynamics and conjugate gradients.
Reviews of Modern Physics, 64(4):1045–1097, Oct 1992.

[26] N. Lorente and M. Persson.
Theoretical aspects of tunneling-current-induced bond excitation and breaking at surfaces.
Faraday Discussions, 117:277–290, 2000.

[27] A. Kirakosian, M.J. Comstock, J. Cho, and M.F. Crommie.
Molecular commensurability with a surface reconstruction: STM study of azobenzene on Au(111).
Physical Review B, 71(11):113409, 2005.

[28] M. Böhringer, K. Morgenstern, W.D. Schneider, R. Berndt, F. Mauri, A. De Vita, and R. Car.
Two-Dimensional Self-Assembly of Supramolecular Clusters and Chains.
Physical Review Letters, 83(2):324–327, July 1999.

[29] D.D. Chambliss, R.J. Wilson, and S. Chiang.
Nucleation of ordered Ni island arrays on Au(111) by surface-lattice dislocations.
Physical Review Letters, 66(13):1721–1724, Apr 1991.

[30] P. Heimann, H. Neddermeyer, and H.F. Roloff.
Ultraviolet photoemission for intrinsic surface states of the noble metals.
Journal of Physics C, 10(1):L17–L21, 1977.

[31] F. Reinert, G. Nicolay, S. Schmidt, D. Ehm, and S. Hüfner.
Direct measurements of the L-gap surface states on the (111) face of noble metals by photoelectron spectroscopy.
Physical Review B, 63(11):115415, 2001.

[32] W. Chen, V. Madhavan, T. Jamneala, and M.F. Crommie.
Scanning Tunneling Microscopy Observation of an Electronic Superlattice at the Surface of Clean Gold.
Physical Review Letters, 80(7):1469–1472, Feb 1998.

[33] J.K. Gimzewski, E. Stoll, and R.R. Schlittler.
Scanning tunneling microscopy of individual molecules of copper phthalocyanine adsorbed on polycrystalline silver surfaces.
Surface Science, 181(1-2):267–277, 1987.

[34] P.H. Lippel, R.J. Wilson, M.D. Miller, Ch. Wöll, and S. Chiang.
High-Resolution Imaging of Copper-Phthalocyanine by Scanning-Tunneling Microscopy.
Physical Review Letters, 62(2):171–174, Jan 1989.

[35] H. Ohtani, R.J. Wilson, S. Chiang, and C.M. Mate.
Scanning Tunneling Microscopy Observations of Benzene Molecules on the Rh(111)-(3 × 3) (C_6H_6 + 2CO) Surface.
Physical Review Letters, 60(23):2398–2401, Jun 1988.

[36] L. Bartels, G. Meyer, and K.H. Rieder.
Controlled vertical manipulation of single CO molecules with the scanning tunneling microscope: A route to chemical contrast.
Applied Physics Letters, 71:213, 1997.

[37] J.A. Stroscio and D.M. Eigler.
Atomic and Molecular Manipulation with the Scanning Tunneling Microscope.
Science, 254(5036):1319–1326, 1991.

[38] P. Sautet and M.L. Bocquet.
STM and chemistry: A qualitative molecular orbital understanding of the image of CO on a Pt surface.
Surface Science, 360(1):128–136, 1996.

[39] J. Repp, G. Meyer, S.M. Stojković, A. Gourdon, and C. Joachim.
Molecules on Insulating Films: Scanning-Tunneling Microscopy Imaging of Individual Molecular Orbitals.
Physical Review Letters, 94(2):26803, 2005.

[40] S. Zöphel.
Adsorptionsplatzbestimmungen auf der Cu(211)-Oberflaeche und Manipulation von Atomen und Molekülen mit dem Tieftemperatur-Rastertunnelmikroskop.
PhD thesis, Freie Universität Berlin, 1996.

[41] M. Alemani.
Low Temperature STM Investigation of Molecular Manipulation, Decoupling, and Switching.
PhD thesis, Freie Universität Berlin, 2006.

[42] I. Horcas, R. Fernández, J.M. Gómez-Rodríguez, J. Colchero, J. Gómez-Herrero, and A.M. Baró.
WSXM: A software for scanning probe microscopy and a tool for nanotechnology.
Review of Scientific Instruments, 78:013705, 2007.

[43] A.I. Day, R.J. Blanch, A.P. Arnold, S. Lorenzo, G.R. Lewis, and I. Dance.
A cucurbituril-based gyroscane: a new supramolecular form.
Angewandte Chemie International Edition, 41(2):275–277, 2002.

[44] W.A. Freeman.
Structures of the p-xylylenediammonium chloride and calcium hydrogensulfate adducts of the cavitand 'cucurbituril', $C_{36}H_{36}N_{24}O_{12}$.
Acta Crystallographica B, 40(4):382–387, 1984.

[45] R.G. Hicks, M.T. Lemaire, L. Öhrström, J.F. Richardson, L.K. Thompson, and Z. Xu.
Strong Supramolecular-Based Magnetic Exchange in-Stacked Radicals. Structure and Magnetism of a Hydrogen-Bonded Verdazyl Radical: Hydroquinone Molecular Solid.
Journal of the American Chemical Society, 123(29):7154–7159, 2001.

[46] M.E. Williams, K.D. Benkstein, C. Abel, P.H. Dinolfo, and J.T. Hupp.
Shape-Selective Transport through Rectangle-Based Molecular Materials: Thin-Film Scanning Electrochemical Microscopy Studies.
Proceedings of the National Academy of Sciences of the United States of America, 99(8):5171–5177, 2002.

[47] G.M. Whitesides and R.F. Ismagilov.
Complexity in Chemistry.
Science, 284(5411):89–92, 1999.

[48] E.I. Altman and R.J. Colton.
Determination of the orientation of C_{60} adsorbed on Au(111) and Ag(111).
Physical Review B, 48(24):18244–18249, 1993.

[49] C. Rogero, J.I. Pascual, J. Gómez-Herrero, and A.M. Baró.
Resolution of site-specific bonding properties of C_{60} adsorbed on Au(111).
Journal of Chemical Physics, 116(2):832–836, 2002.

[50] M.K.J. Johansson, S.M. Gray, L.S.O. Johansson, A.J. Maxwell, and P.A. Bruhwiler.
Adsorption of C_{60} on Al(111) studied with scanning tunnelling microscopy.
Surface Science, 397(1):314–321, 1998.

[51] S. Clair, S. Pons, A.P. Seitsonen, H. Brune, K. Kern, and J.V. Barth.
STM Study of Terephthalic Acid Self-Assembly on Au(111): Hydrogen-Bonded Sheets on an Inhomogeneous Substrate.
Journal of Physical Chemistry B, 108(38):14585–14590, 2004.

[52] S. Griessl, M. Lackinger, M. Edelwirth, M. Hietschold, and W.M. Heckl.
Self-Assembled Two-Dimensional Molecular Host-Guest Architectures From Trimesic Acid.
Single Molecules, 3(1):25–31, 2002.

[53] T. Kawai, H. Tanaka, and T. Nakagawa.
Low dimensional self-organization of DNA-base molecules on Cu(111) surfaces.
Surface Science, 386(1):124–136, 1997.

[54] N. Lin, D. Payer, A. Dmitriev, T. Strunskus, C. Wöll, J.V. Barth, and K. Kern.
Two-Dimensional Adatom Gas Bestowing Dynamic Heterogeneity on Surfaces.
Angewandte Chemie International Edition, 44(10):1488–1491, 2005.

[55] J.A. Theobald, N.S. Oxtoby, M.A. Phillips, N.R. Champness, and P.H. Beton.
Controlling molecular deposition and layer structure with supramolecular surface assemblies.
Nature, 424:1029–1031, 2003.

[56] T. Livneh, Y. Lilach, and M. Asscher.
Dipole-dipole interactions among CH_3Cl molecules on Ru(001): Correlation between work function change and thermal desorption studies.
Journal of Chemical Physics, 111:11138–11146, December 1999.

[57] E. Bauer and H. Poppa.
Recent Advances in Epitaxy.
Thin Solid Films, 12(1):167–185, 1972.

[58] B.J. Hinch and L.H. Dubois.
Water adsorption of Cu(111): evidence for Volmer-Weber film growth.
Chemical Physics Letters, 181(1):10–15, 1991.

[59] J.S. Yang, C.P. Liu, B.C. Lin, C.W. Tu, and G.H. Lee.
Solid-State Molecular Folding and Supramolecular Structures of Triptycene-Derived Secondary Dicarboxamides.
The Journal of Organic Chemistry, 67(21):7343–7354, 2002.

[60] D.M. Guldi, C. Luo, M. Prato, A. Troisi, F. Zerbetto, M. Scheloske, E. Dietel, W. Bauer, and A. Hirsch.
Parallel (face-to-face) versus perpendicular (edge-to-face) alignment of electron donors and acceptors in fullerene porphyrin dyads: the importance of orientation in electron transfer.
Journal of the American Chemical Society, 123(37):9166–7, 2001.

[61] S. Tsuzuki, K. Honda, T. Uchimaru, M. Mikami, and K. Tanabe.
Origin of attraction and directionality of the *pi/pi* interaction: model chemistry calculations of benzene dimer interaction.
Journal of the American Chemical Society, 124(1):104–112, 2002.

[62] N.L. Allinger, Y.H. Yuh, and J.H. Lii.
Molecular mechanics. The MM3 force field for hydrocarbons. 1.
Journal of the American Chemical Society, 111(23):8551–8566, 1989.

[63] J.H. Lii and N.L. Allinger.
Molecular mechanics. The MM3 force field for hydrocarbons. 2. Vibrational frequencies and thermodynamics.
Journal of the American Chemical Society, 111(23):8566–8575, 1989.

[64] N.L. Allinger, Z.Q.S. Zhu, and K. Chen.
Molecular mechanics (MM3) studies of carboxylic acids and esters.
Journal of the American Chemical Society, 114(15):6120–6133, 1992.

[65] P. Ordejón, E. Artacho, and J.M. Soler.
Self-consistent order-N density-functional calculations for very large systems.
Physical Review B, 53(16):R10441–R10444, Apr 1996.

[66] D. Sánchez-Portal, P. Ordejón, E. Artacho, and J.M. Soler.
Density-functional method for very large systems with LCAO basis sets.
International Journal of Quantum Chemistry, 65(5):453–461, 1997.

[67] D. Bonifazi, H. Spillmann, A. Kiebele, M. de Wild, P. Seiler, C. Fuyong, H.J. Güntherodt, Jung T.A., and F. Diederich.

Supramolecular patterned surfaces driven by cooperative assembly of C_{60} and porphyrins on metal substrates.
Angewandte Chemie International Edition, 43:4759–4763, 2004.

[68] M. de Wild, S. Berner, H. Suzuki, H. Yanagi, D. Schlettwein, S. Ivan, A. Baratoff, H.J. Guentherodt, and T.A. Jung.
A Novel Route To Molecular Self-Assembly: Self-Intermixed Monolayer Phases.
ChemPhysChem, 3(10):881–885, 2002.

[69] J.K. Gimzewski, T.A. Jung, M.T. Cuberes, and R.R. Schlittler.
Scanning tunneling microscopy of individual molecules: Beyond imaging.
Surface Science, 386(1):101–114, 1997.

[70] H. Spillmann, A. Kiebele, M. Stohr, T.A. Jung, D. Bonifazi, F. Cheng, and F. Diederich.
A two-dimensional porphyrin-based porous network featuring communicating cavities for the templated complexation of fullerenes.
Advanced materials, 18(3):275–279, 2006.

[71] K.J. Franke, G. Schulze, N. Henningsen, I. Fernández-Torrente, J.I. Pascual, S. Zarwell, K. Rück-Braun, M. Cobian, and N. Lorente.
Reducing the Molecule-Substrate Coupling in C_{60}-Based Nanostructures by Molecular Interactions.
Physical Review Letters, 100(3):36807, 2008.

[72] T. Frederiksen, K.J. Franke, A. Arnau, G. Schulze, J.I. Pascual, and N. Lorente.
Dynamic Jahn-Teller effect in electron transport through single C_{60} mole cules .
Arxiv preprint cond-mat/arXiv:0804.3415v1, 2008.

[73] Y. Wang, R. Yamachika, A. Wachowiak, M. Grobis, and M.F. Crommie.
Tuning fulleride electronic structure and molecular ordering via variable layer index.
Nature Materials, 7:194, 2008.

[74] D.M. Duffy and A.M. Stoneham.
Conductivity and 'negative U' for ionic grain boundaries.
Journal of Physics C, 16(21):4087–4092, 1983.

[75] K.J. Miller and J. Savchik.
A new empirical method to calculate average molecular polarizabilities.
Journal of the American Chemical Society, 101(24):7206–7213, 1979.

[76] K.D. Bonin and V.V. Kresin.
Electric-dipole Polarizabilities of Atoms, Molecules, and Clusters.
World Scientific, 1997.

[77] R. Hesper, L.H. Tjeng, and G.A. Sawatzky.
Strongly reduced band gap in a correlated insulator in close proximity to a metal.
Europhysics Letters, 40(2):177–182, 1997.

[78] H.W. Kroto, J.R. Heath, S.C. O'Brien, R.F. Curl, and R.E. Smalley.
C_{60}: Buckminsterfullerene.
Nature, 318:162–163, 1985.

[79] E.I. Altman and R.J. Colton.
The interaction of C_{60} with noble metal surfaces.
Surface science, 295(1-2):13–33, 1993.

[80] E.I. Altman and R.J. Colton.
Nucleation, growth, and structure of fullerene films on Au(111).
Surface science, 279(1-2):49–67, 1992.

[81] R. Gaisch, R. Berndt, J.K. Gimzewski, B. Reihl, R.R. Schlittler, W.D. Schneider, and M. Tschudy.
Internal structure of C_{60} fullerence molecules as revealed by low-temperature STM.
Applied Physics A, 57(2):207–210, 1993.

[82] G. Schull and R. Berndt.
Orientationally Ordered (7×7) Superstructure of C_{60} on Au(111).
Physical Review Letters, 99:226105, 2007.

[83] M. Grobis, A. Wachowiak, R. Yamachika, and M.F. Crommie.
Tuning negative differential resistance in a molecular film.
Applied Physics Letters, 86:204102, 2005.

[84] B.W. Hoogenboom, R. Hesper, L.H. Tjeng, and G.A. Sawatzky.
Charge transfer and doping-dependent hybridization of C_{60} on noble metals.
Physical Review B, 57(19):11939–11942, May 1998.

[85] X. Lu, M. Grobis, K.H. Khoo, S.G. Louie, and M.F. Crommie.
Charge transfer and screening in individual C_{60} molecules on metal substrates: A scanning tunneling spectroscopy and theoretical study.
Physical Review B, 70(11):115418, Sep 2004.

[86] T.R. Ohno, Y. Chen, S.E. Harvey, G.H. Kroll, J.H. Weaver, R.E. Haufler, and R.E. Smalley.
C_{60} bonding and energy-level alignment on metal and semiconductor surfaces.
Physical Review B, 44(24):13747–13755, Dec 1991.

[87] C. Silien, N.A. Pradhan, W. Ho, and P.A. Thiry.
Influence of adsorbate-substrate interaction on the local electronic structure of C_{60} studied by low-temperature STM.
Physical Review B, 69(11):115434, Mar 2004.

[88] C.T. Tzeng, W.S. Lo, J.Y. Yuh, R.Y. Chu, and K.D. Tsuei.
Photoemission, near-edge x-ray-absorption spectroscopy, and low-energy electron-diffraction study of C_{60} on Au(111) surfaces.
Physical Review B, 61(3):2263–2272, Jan 2000.

[89] G. Schulze, K.J. Franke, and J.I. Pascual.
Resonant heating and substrate-mediated cooling of a single C_{60} molecule in a tunnel junction.
Arxiv preprint cond-mat/arXiv:0803.2222v1, 2008.

[90] J.I. Pascual, J. Gómez-Herrero, D. Sánchez-Portal, and H.P. Rust.
Vibrational spectroscopy on single C_{60} molecules: The role of molecular orientation.

The Journal of Chemical Physics, 117(21):9531–9534, 2002.

[91] J. De Vries, H. Steger, B. Kamke, C. Menzel, B. Weisser, W. Kamke, and I.V. Hertel.
Single-photon ionization of C_{60} fullerene and C_{70} fullerene with synchrotron radiation-determination of the ionization potential of C_{60}.
Chemical Physics Letters, 188(3-4):159–162, JAN 10 1992.

[92] I.V. Hertel, H. Steger, J. de Vries, B. Weisser, C. Menzel, B. Kamke, and W. Kamke.
Giant plasmon excitation in free C_{60} and C_{70} molecules studied by photoionization.
Physical Review Letters, 68(6):784–787, Feb 1992.

[93] D.L. Lichtenberger, K.W. Nebesny, C.D. Ray, D.R. Huffman, and L.D. Lamb.
Valence and core photoelectron-spectroscopy of C_{60}, buckminsterfullerene.
Chemical Physics Letters, 176(2):203–208, JAN 11 1991.

[94] R.K. Yoo, B. Ruscic, and J. Berkowitz.
Vacuum ultraviolet photoionization mass-spectrometric study of C_{60}.
Journal of Chemical Physics, 96(2):911–918, January 1992.

[95] S.H. Yang, C.L. Pettiette, J. Conceicao, O. Cheshnovsky, and R.E. Smalley.
UPS of buckminsterfullerene and other large clusters of carbon.
Chemical Physics Letters, 139(3-4):233–238, 1987.

[96] R. Hesper.
The influence of surfaces and interfaces on the properties of C_{60} compounds.
PhD thesis, Rijksuniversiteit Groningen, 2000.

[97] D.V. Konarev, Y.V. Zubavichus, E.F. Valeev, Y.L. Slovokhotov, Y.M. Shul'ga, and R.N. Lyubovskay.
C_{60} complexes with dianthracene and triptycene: synthesis and crystal structures.
Synthetic Metals, 103(1-3):2364–2365, 1999.

[98] J.I. Pascual.
Propiedades electrónicas de sistemas nanométricos.
PhD thesis, Universidad Autónoma de Madrid, 1998.

[99] M. Grobis, X. Lu, and M.F. Crommie.
Local electronic properties of a molecular monolayer: C_{60} on Ag(001).
Physical Review B, 66(16):161408, Oct 2002.

[100] N. Toyota, M. Lang, and J. Müller.
Low-dimensional molecular metals.
Springer, 2007.

[101] J. Ferraris, D.O. Cowan, V. Walatka Jr, and J.H. Perlstein.
Electron transfer in a new highly conducting donor-acceptor complex.
Journal of the American Chemical Society, 95(3):948–949, 1973.

[102] L.B. Coleman, M.J. Cohen, D.J. Sandman, F.G. Yamagishi, A.F. Garito, and A.J. Heeger.
Superconducting fluctuations and the Peierls instability in an organic solid.

Solid State Communications, 12(11):1125–1132, 1973.

[103] G.A. Thomas, D.E. Schafer, F. Wudl, P.M. Horn, D. Rimai, J.W. Cook, D.A. Glocker, M.J. Skove, C.W. Chu, R.P. Groff, J.L. Gillson, R.C. Wheland, L.R. Melby, M.B. Salamon, R.A. Craven, G. De Pasquali, A.N. Bloch, D.O. Cowan, V.V. Walatka, R.E. Pyle, R. Gemmer, T.O. Poehler, G.R. Johnson, M.G. Miles, J.D. Wilson, J.P. Ferraris, and T.F. Finnegan.
Electrical conductivity of tetrathiafulvalenium-tetracyanoquinodimethanide (TTF-TCNQ).
Physical Review B, 13(11):5105–5110, Jun 1976.

[104] T. Nishiguchi, M. Kageshima, N. Ara-Kato, and A. Kawazu.
Behavior of Charge Density Waves in a One-Dimensional Organic Conductor Visualized by Scanning Tunneling Microscopy.
Physical Review Letters, 81(15):3187–3190, 1998.

[105] M. Sing, U. Schwingenschlögl, R. Claessen, P. Blaha, J.M.P. Carmelo, L.M. Martelo, P.D. Sacramento, M. Dressel, and C.S. Jacobsen.
Electronic structure of the quasi-one-dimensional organic conductor TTF-TCNQ.
Physical Review B, 68(12):125111, 2003.

[106] K. Murata, S. Kagoshima, S. Yasuzuka, H. Yoshimo, and R. Kondo.
High-Pressure Research in Organic Conductors.
Journal of the Physical Society of Japan, 75(5):051015–051015, 2006.

[107] A.J. Berlinsky, J.F. Carolan, and L. Weiler.
Photoelectron Spectrum and Electronic Structure of Tetrathiofulvalene (TTF).
Canadian Journal of Chemistry, 52(19):3373–3377, 1974.

[108] E.M. Engler, F.B. Kaufman, D.C. Green, C.E. Klots, and R.N. Compton.
Ionization potentials and donor properties of selenium analogs of tetrathiafulvalene.
Journal of the American Chemical Society, 97(10):2921–2922, 1975.

[109] M. Bendikov, F. Wudl, and D.F. Perepichka.
Tetrathiafulvalenes, oligoacenenes, and their buckminsterfullerene derivatives: the brick and mortar of organic electronics.
Chemical Reviews, 104(11):4891–4946, 2004.

[110] F. Wudl, G.M. Smith, and E.J. Hufnagel.
Bis-1,3-dithiolium chloride: an unusually stable organic radical cation.
Journal of the Chemical Society D, 1970(21):1453–1454, 1970.

[111] R.N. Compton, P.W. Reinhardt, and C.D. Cooper.
Collisional ionization of Na, K, and Cs by CO_2, COS, and CS_2: Molecular electron affinities.
The Journal of Chemical Physics, 63(9):3821–3827, 1975.

[112] R.N. Compton and C.D. Cooper.
Negative ion properties of tetracyanoquinodimethan: Electron affinity and compound states.
The Journal of Chemical Physics, 66:4325, 1977.

[113] C.E. Klots, R.N. Compton, and V.F. Raaen.
Electronic and ionic properties of molecular TTF and TCNQ.
The Journal of Chemical Physics, 60:1177, 2003.

[114] A.L. Smith and P. Tan.
Creatine synthesis: An undergraduate organic chemistry laboratory experiment.
Journal of chemical education, 83(11):1654–1657, 2006.

[115] B. Milián, R. Pou-Amérigo, R. Viruela, and E. Ortí.
On the electron affinity of TCNQ.
Chemical Physics Letters, 391(1-3):148–151, 2004.

[116] E. Faulques, A. Leblanc, P. Molinié, M. Decoster, F. Conana, J.E. Guerchais, and J. Sala-Pala.
Determination of a charge transfer in molybdenum complexes of 7,7,8,8,-tetracyano-p-quinodimethane with vibrational spectroscopy.
Spectrochimica Acta, 51A:805–819, 1995.

[117] T.J. Kistenmacher, T.E. Phillips, and D.O. Cowan.
The crystal structure of the 1:1 radical cation-radical anion salt of 2,2'-bis-l,3-dithiole (TTF) and 7,7,8,8-tetracyanoquinodimethane (TCNQ).
Structural Crystallography and Crystal Chemistry, 30(3):763–768, 1974.

[118] N. Ara, A. Kawazu, H. Shigekawa, K. Yase, and M. Yoshimura.
Structural studies of tetrathiafulvalene–tetracyanoquinodimethane thin films by scanning tunneling microscopy.
Applied Physics Letters, 66(24):3278, 1995.

[119] D. Jerome.
Organic conductors: from charge density wave TTF-TCNQ to superconducting $(TMTSF)_2PF_6$.
Chemical reviews, 104(11):5565–92, 2004.

[120] S.K. Khanna, J.P. Pouget, R. Comes, A.F. Garito, and A.J. Heeger.
X-ray studies of $2k_F$ and $4k_F$ anomalies in tetrathiafulvalene-tetracyanoquinodimethane (TTF-TCNQ).
Physical Review B, 16(4):1468–1479, Aug 1977.

[121] J. Fraxedas, Y.J. Lee, I. Jiménez, R. Gago, R.M. Nieminen, P. Ordejón, and E. Canadell.
Characterization of the unoccupied and partially occupied states of TTF-TCNQ by XANES and first-principles calculations.
Physical Review B, 68(19):195115, 2003.

[122] S. Ishibashi and M. Kohyama.
Ab initio pseudopotential calculation for TTF-TCNQ and TSeF-TCNQ.
Physical Review B, 62(12):7839–7844, 2000.

[123] F. Zwick, D. Jérome, G. Margaritondo, M. Onellion, J. Voit, and M. Grioni.
Band Mapping and Quasiparticle Suppression in the One-Dimensional Organic Conductor TTF-TCNQ.
Physical Review Letters, 81(14):2974–2977, 1998.

[124] R. Comès, S.M. Shapiro, G. Shirane, A.F. Garito, and A.J. Heeger.
Neutron-Scattering Study of the 38- and 54-K Phase Transitions in Deuterated Tetrathiafulvalene- Tetracyanoquinodimethane (TTF-TCNQ).
Physical Review Letters, 35(22):1518–1521, Dec 1975.

[125] F. Denoyer, F. Comès, A.F. Garito, and A.J. Heeger.
X-Ray-Diffuse-Scattering Evidence for a Phase Transition in Tetrathiafulvalene Tetracyanoquinodimethane (TTF-TCNQ).
Physical Review Letters, 35(7):445–449, Aug 1975.

[126] Z.Z. Wang, J.C. Girard, C. Pasquier, D. Jérome, and K. Bechgaard.
Scanning tunneling microscopy in TTF-TCNQ: Phase and amplitude modulated charge density waves.
Physical Review B, 67(12):121401, 2003.

[127] W.J. Gunning, C.K. Chiang, A.J. Heeger, and A.J. Epstein.
Effects of controlled disorder on the phase-transitions and charge-density wave state in tetrathiofulvalene-tetracyanoquinodimethane.
Physica Status Solidi (b), 96(1):145–151, 1979.

[128] T. Takahashi, D. Jérome, F. Masin, J.M. Fabre, and L. Giral.
^{13}C NMR studies of TTF(^{13}C)-TCNQ.
Journal of Physics C, 17(21):3777–3792, 1984.

[129] J. Fraxedas, S. Molas, A. Figueras, I. Jiménez, R. Gago, P. Auban-Senzier, and M. Goffman.
Thin Films of Molecular Metals TTF-TCNQ.
Journal of Solid State Chemistry, 168(2):384–389, 2002.

[130] R. Hoffmann.
A chemical and theoretical way to look at bonding on surfaces.
Reviews of Modern Physics, 60(3):601–628, Jul 1988.

[131] J.V. Barth, G. Costantini, and K. Kern.
Engineering atomic and molecular nanostructures at surfaces.
Nature, 437(7059):671–679, 2005.

[132] J.V. Barth, H. Brune, G. Ertl, and R.J. Behm.
Scanning tunneling microscopy observations on the reconstructed Au(111) surface: Atomic structure, long-range superstructure, rotational domains, and surface defects.
Physical Review B, 42(15):9307–9318, Nov 1990.

[133] N. Knorr, H. Brune, M. Epple, A. Hirstein, M.A. Schneider, and K. Kern.
Long-range adsorbate interactions mediated by a two-dimensional electron gas.
Physical Review B, 65(11):115420, 2002.

[134] H. Brune, M. Giovannini, K. Bromann, and K. Kern.
Self-organized growth of nanostructure arrays on strain-relief patterns.
Nature, 394:451, 1998.

[135] K. Pohl, M.C. Bartelt, J. de la Figuera, N.C. Bartelt, J. Hrbek, and R.Q. Hwang.
Identifying the forces responsible for self-organization of nanostructures at crystal surfaces.

Nature, 397(6716):238–241, 1999.

[136] F. Couthon, E. Clottes, C. Vial, R. Tan, V. Osman, G. Tan, and H. Ibach.
The role of surface stress in reconstruction, epitaxial growth and stabilization of mesoscopic structures.
Surface Science Reports, 29(5):195–263, 1997.

[137] D.J. Keller, H.M. McConnell, and V.T. Moy.
Theory of superstructures in lipid monolayer phase transitions.
The Journal of Physical Chemistry, 90(11):2311–2315, 1986.

[138] P. Hyldgaard and M. Persson.
Long-ranged adsorbate-adsorbate interactions mediated by a surface-state band.
Journal of Physics: Condensed Matter, 12(1):L13–L19, 2000.

[139] J. Repp, F. Moresco, G. Meyer, K.H. Rieder, P. Hyldgaard, and M. Persson.
Substrate Mediated Long-Range Oscillatory Interaction between Adatoms: Cu/Cu(111).
Physical Review Letters, 85(14):2981–2984, 2000.

[140] S. Lukas, G. Witte, and Ch. Wöll.
Novel Mechanism for Molecular Self-Assembly on Metal Substrates: Unidirectional Rows of Pentacene on Cu(110) Produced by a Substrate-Mediated Repulsion.
Physical Review Letters, 88(2):028301, Dec 2001.

[141] F. Silly, M. Pivetta, M. Ternes, F. Patthey, J.P. Pelz, and W.D. Schneider.
Creation of an Atomic Superlattice by Immersing Metallic Adatoms in a Two-Dimensional Electron Sea.
Physical Review Letters, 92(1):16101, 2004.

[142] M. Ternes, C. Weber, M. Pivetta, F. Patthey, J.P. Pelz, T. Giamarchi, F. Mila, and W.D. Schneider.
Scanning-Tunneling Spectroscopy of Surface-State Electrons Scattered by a Slightly Disordered Two-Dimensional Dilute "Solid": Ce on Ag (111).
Physical Review Letters, 93(14):146805, 2004.

[143] S.U. Nanayakkara, E.C.H. Sykes, L.C. Fernández-Torres, M.M. Blake, and P.S. Weiss.
Long-Range Electronic Interactions at a High Temperature: Bromine Adatom Islands on Cu(111).
Physical Review Letters, 98(20):206108, 2007.

[144] T. Yokoyama, T. Takahashi, K. Shinozaki, and M. Okamoto.
Quantitative Analysis of Long-Range Interactions between Adsorbed Dipolar Molecules on Cu(111).
Physical Review Letters, 98(20):206102, 2007.

[145] L.L. Wang and H.P. Cheng.
Density functional study of the adsorption of a C_{60} monolayer on Ag(111) and Au(111) surfaces.
Physical Review B, 69(16):165417, Apr 2004.

[146] N. Lorente, M.F.G. Hedouin, R.E. Palmer, and M. Persson.
Chemisorption of benzene and STM dehydrogenation products on Cu(100).
Physical Review B, 68(15):155401, Oct 2003.

[147] K. Huang.
Statistical mechanics.
Wiley New York, 1987.

[148] R. Baierlein.
Thermal Physics.
Cambridge University Press, 1999.

[149] E. Wigner.
On the Interaction of Electrons in Metals.
Physical Review, 46(11):1002–1011, Dec 1934.

[150] F. Wennmohs, V. Staemmler, and M. Schindler.
Theoretical investigation of weak hydrogen bonds to sulfur.
The Journal of Chemical Physics, 119:3208, 2003.

[151] S.C. Glotzer, D. Stauffer, and N. Jan.
Monte Carlo simulations of phase separation in chemically reactive binary mixtures.
Physical Review Letters, 72(26):4109–4112, Jun 1994.

[152] C. Sagui and R.C. Desai.
Kinetics of topological defects in systems with competing interactions.
Physical Review Letters, 71(24):3995–3998, Dec 1993.

[153] L. Romaner, G. Heimel, J.L. Brédas, A. Gerlach, F. Schreiber, R.L. Johnson, J. Zegenhagen, S. Duhm, N. Koch, and E. Zojer.
Impact of Bidirectional Charge Transfer and Molecular Distortions on the Electronic Structure of a Metal-Organic Interface.
Physical Review Letters, 99(25):256801, 2007.

[154] M. Hippler.
Quantum chemical study and infrared spectroscopy of hydrogen-bonded $CHCl_3$–NH_3 in the gas phase.
The Journal of Chemical Physics, 127(8):084306, 2007.

[155] J.Y. Park, U.D. Ham, S.J. Kahng, Y. Kuk, K. Miyake, K. Hata, and H. Shigekawa.
Modification of surface-state dispersion upon Xe adsorption: A scanning tunneling microscope study.
Physical Review B, 62(24):R16341–R16344, Dec 2000.

[156] F. Forster, G. Nicolay, F. Reinert, D. Ehm, S. Schmidt, and S. Hüfner.
Surface and interface states on adsorbate covered noble metal surfaces.
Surface science, 532:160–165, 2003.

[157] T. Andreev, I. Barke, and H. Hövel.
Adsorbed rare-gas layers on Au(111): Shift of the Shockley surface state studied with ultraviolet photoelectron spectroscopy and scanning tunneling spectroscopy.

Physical Review B, 70(20):205426, 2004.

[158] J. Repp, G. Meyer, and K.H. Rieder.
Snell's Law for Surface Electrons: Refraction of an Electron Gas Imaged in Real Space.
Physical Review Letters, 92(3):036803, Jan 2004.

[159] N. Nicoara, E. Román, J.M. Gómez-Rodríguez, J.A. Martín-Gago, and J. Méndez.
Scanning tunneling and photoemission spectroscopies at the PTCDA/Au (111) interface.
Organic Electronics, 7(5):287–294, 2006.

[160] A. Hotzel, G. Moos, K. Ishioka, M. Wolf, and G. Ertl.
Femtosecond electron dynamics at adsorbate-metal interfaces and the dielectric continuum model.
Applied Physics B, 68(3):615–622, 1999.

[161] N.V. Smith.
Phase analysis of image states and surface states associated with nearly-free-electron band gaps.
Physical Review B, 32(6):3549–3555, Sep 1985.

[162] K. Morgenstern, K.F. Braun, and K.H. Rieder.
Surface-State Depopulation on Small Ag(111) Terraces.
Physical Review Letters, 89(22):226801, Nov 2002.

[163] S.D. Kevan and R.H. Gaylord.
High-resolution photoemission study of the electronic structure of the noble-metal (111) surfaces.
Physical Review B, 36(11):5809–5818, Oct 1987.

[164] Y. Hasegawa and Ph. Avouris.
Direct observation of standing wave formation at surface steps using scanning tunneling spectroscopy.
Physical Review Letters, 71(7):1071–1074, Aug 1993.

[165] C.D. Lindstrom, M. Muntwiler, and X.Y. Zhu.
Electron Transport Across the Alkanethiol Self-assembled Monolayer/Au (111) Interface: Role of the Chemical Anchor.
Journal of Physical Chemistry B, 109(46):21492–21495, 2005.

[166] R. Temirov, S. Soubatch, A. Luican, and F.S. Tautz.
Free-electron-like dispersion in an organic monolayer film on a metal substrate.
Nature, 444(7117):350–353, 2006.

[167] N.W. Ashcroft and N.D. Mermin.
Solid state physics.
Saunders College Philadelphia, Pa, 1976.

[168] C. Kittel et al.
Introduction to solid state physics.
Wiley New York, 1986.

[169] Y. Tomkiewicz, B.A. Scott, L.J. Tao, and R.S. Title.
Magnetic Studies of Tetrathiofulvalinium Tetracyanoquinodimethanide (TTF-TCNQ).
Physical Review Letters, 32(24):1363–1366, Jun 1974.

[170] J.B. Torrance, Y. Tomkiewicz, and B.D. Silverman.
Enhancement of the magnetic susceptibility of TTF-TCNQ (tetrathiafulvalene-tetracyanoquinodimethane) by Coulomb correlations.
Physical Review B, 15(10):4738–4749, May 1977.

[171] M. Johnson and J. Clarke.
Spin-polarized scanning tunneling microscope: Concept, design, and preliminary results from a prototype operated in air.
Journal of Applied Physics, 67:6141, 1990.

[172] R. Wiesendanger, H.J. Güntherodt, G. Güntherodt, R.J. Gambino, and R. Ruf.
Observation of vacuum tunneling of spin-polarized electrons with the scanning tunneling microscope.
Physical Review Letters, 65(2):247–250, Jul 1990.

[173] P.W. Anderson.
Ground State of a Magnetic Impurity in a Metal.
Physical Review, 164(2):352–359, Dec 1967.

[174] W.G. van der Wiel, S.D. Franceschi, T. Fujisawa, J.M. Elzerman, S. Tarucha, and L.P. Kouwenhoven.
The Kondo Effect in the Unitary Limit.
Science, 289(5487):2105, 2000.

[175] D. Goldhaber-Gordon, J. Göres, M.A. Kastner, H. Shtrikman, D. Mahalu, and U. Meirav.
From the Kondo Regime to the Mixed-Valence Regime in a Single-Electron Transistor.
Physical Review Letters, 81(23):5225–5228, 1998.

[176] K. Nagaoka, T. Jamneala, M. Grobis, and M.F. Crommie.
Temperature Dependence of a Single Kondo Impurity.
Physical Review Letters, 88(7):077205, Feb 2002.

[177] J.J. Parks, A.R. Champagne, G.R. Hutchison, S. Flores-Torres, H.D. Abruña, and D.C. Ralph.
Tuning the Kondo Effect with a Mechanically Controllable Break Junction.
Physical Review Letters, 99(2):026601, 2007.

[178] J.W. Gadzuk and M. Plihal.
Introductory Lecture. Excited states at surfaces: Fano profiles in STM spectroscopy of adsorbates.
Faraday Discussions, 117:1–13, 2000.

[179] V. Iancu, A. Deshpande, and S.W. Hla.
Manipulating kondo temperature via single molecule switching.
Nano letters, 6(4):820–823, 2006.

[180] V. Iancu, A. Deshpande, and S.W. Hla.
Manipulation of the Kondo Effect via Two-Dimensional Molecular Assembly.
Physical Review Letters, 97(26):266603, 2006.

[181] J. Li, W.D. Schneider, R. Berndt, and B. Delley.
Kondo Scattering Observed at a Single Magnetic Impurity.
Physical Review Letters, 80(13):2893–2896, 1998.

[182] V. Madhavan, W. Chen, T. Jamneala, M.F. Crommie, and N.S. Wingreen.
Tunneling into a Single Magnetic Atom: Spectroscopic Evidence of the Kondo Resonance.
Science, 280(5363):567, 1998.

[183] N. Neel, J. Kroeger, L. Limot, K. Palotas, W.A. Hofer, and R. Berndt.
Conductance and Kondo effect of a controlled single atom contact.
Arxiv preprint cond-mat/0610419, 2006.

[184] R. Temirov, A. Lassise, F.B. Anders, and F.S. Tautz.
Kondo effect by controlled cleavage of a single-molecule contact.
Nanotechnology, 19(065401):065401, 2008.

[185] P. Wahl, L. Diekhöner, M.A. Schneider, L. Vitali, G. Wittich, and K. Kern.
Kondo Temperature of Magnetic Impurities at Surfaces.
Physical Review Letters, 93(17):176603, 2004.

[186] P. Wahl, L. Diekhöner, G. Wittich, L. Vitali, M.A. Schneider, and K. Kern.
Kondo Effect of Molecular Complexes at Surfaces: Ligand Control of the Local Spin Coupling.
Physical Review Letters, 95(16):166601, 2005.

[187] A. Zhao, Q. Li, L. Chen, H. Xiang, W. Wang, S. Pan, B. Wang, X. Xiao, J. Yang, J.G. Hou, and Q. Zhu.
Controlling the Kondo Effect of an Adsorbed Magnetic Ion Through Its Chemical Bonding.
Science, 309(5740):1542–1544, 2005.

[188] U. Fano.
Effects of Configuration Interaction on Intensities and Phase Shifts.
Physical Review, 124(6):1866–1878, Dec 1961.

[189] J.G. Kushmerick, J. Lazorcik, C.H. Patterson, R. Shashidhar, D.S. Seferos, and G.C. Bazan.
Vibronic contributions to charge transport across molecular junctions.
Nano Letters, 4:639–642, 2004.

[190] H. Park, J. Park, A.K.L. Lim, E.H. Anderson, A.P. Alivisatos, and P.L. McEuen.
Nanomechanical oscillations in a single-C_{60} transistor.
Nature, 407:57, 2000.

[191] B.C. Stipe, M.A. Rezaei, and W. Ho.
Single-Molecule Vibrational Spectroscopy and Microscopy.
Science, 280(5370):1732, 1998.

[192] W. Wang, T. Lee, I. Kretzschmar, and M.A. Reed.
Inelastic electron tunneling spectroscopy of an alkanedithiol self-assembled monolayer.
Nano Letters, 4(4):643, 2004.

[193] K. Flensberg.
Tunneling broadening of vibrational sidebands in molecular transistors.
Physical Review B, 68(20):205323, Nov 2003.

[194] J. Paaske and K. Flensberg.
Vibrational Sidebands and the Kondo Effect in Molecular Transistors.
Physical Review Letters, 94(17):176801, 2005.

[195] N.O. Lipari, C.B. Duke, R. Bozio, A. Girlando, C. Pecile, and A. Padva.
Electron—molecular-vibration coupling in 7,7,8,8-tetracyano-p-Quinodimethane (TCNQ).
Chemical Physics Letters, 44(2):236–240, 1976.

[196] M.J. Rice, N.O. Lipari, and S. Strässler.
Dimerized Organic Linear-Chain Conductors and the Unambiguous Experimental Determination of Electron-Molecular-Vibration Coupling Constants.
Physical Review Letters, 39(21):1359–1362, 1977.