

Publications since 1976

by Matthias Scheffler

1. *Scheffler, M., K. Kambe, and F. Forstmann*: Energy and angle-resolved photoemission. In: Proc. Int. Symp. on Photoemission. (Eds.) R.F. Willis, B. Feuerbacher, B. Fitton and C. Backx. ESA, Paris 1976, 227.
2. *Jacobi, K., M. Scheffler, K. Kambe, and F. Forstmann*: Angle-resolved photoemission from the p(2x2) oxygen overlayer on Ni(001): Measurements and calculations. Solid State Communications **22**, 17 (1977).
3. *Jacobi, K., M. Scheffler, K. Kambe, and F. Forstmann*: Angle-resolved photoemission of the oxygen overlayer on Ni(001): Part 2 (Experiments) ib.. In: Proc. 7th Int. Vac. Congr. & 3rd Conf. Sol. Surf. (Vienna 1977), 2227.
4. *Scheffler, M., K. Kambe, F. Forstmann, and K. Jacobi*: Angle-resolved photoemission of the oxygen overlayer on Ni(001): Part 1 (Calculations). In: Proc. 7th Int. Vac. Congr. & 3rd Conf. Sol. Surf. (Vienna 1977), 2223.
5. *Horn, K., M. Scheffler, and A.M. Bradshaw*: Photoemission from physisorbed xenon: Evidence for lateral interactions. Phys. Rev. Lett. **41**, 822-825 (1978).
6. *Scheffler, M.*: Winkelauflöste Photoemission von Adsorbatsystemen. Ph.D. thesis, Technische Universität Berlin, Fachbereich Physik (1978).
7. *Scheffler, M., K. Horn, A.M. Bradshaw, and K. Kambe*: Photoemission from physisorbed xenon. Nederlands Tijdschrift voor Vacuumtechniek, **2/3/4**, 85 (1978).
8. *Scheffler, M., K. Kambe, and F. Forstmann*: Angle resolved photoemission from adsorbates: Theoretical considerations of polarization effects and symmetry. Solid State Communications **25**, 93 (1978).
9. *Bradshaw, A.M. and M. Scheffler*: Lateral interactions in adsorbed layers. J. Vac. Sci. Tech. **16**, 447 (1979).
10. *Hoffmann, P., C. v. Muschwitz, K. Horn, K. Jacobi, A.M. Bradshaw, K. Kambe, and M. Scheffler*: Angular-resolved photoemission from an ordered oxygen overlayer on aluminium (111). Surf. Sci. **89**, 327 (1979).
11. *Kambe, K. and M. Scheffler*: Theory of photoexcitation of adsorbates. Surf. Sci. **89**, 262 (1979).
12. *Scheffler, M.*: The influence of lateral interactions on the vibrational spectrum of adsorbed CO. Surf. Sci. **81**, 562 (1979).
13. *Scheffler, M., K. Horn, A.M. Bradshaw, and K. Kambe*: Photoemission from physisorbed xenon. Surf. Sci. **80**, 69 (1979).

14. *Hora, R. and M. Scheffler*: Photoemission and the electronic structure of a c(2x2) adsorbate-layer on Pd. In: Proc. 4th Int. Conf. on Sol. Surf. and the 3rd European Conf. on Surf. Sci., Cannes, France, Supplément à la Revue “Le Vide, les Couches Mincees” N° 201, 1147 (1980).

15. *Bernholc, J., N.O. Lipari, S.T. Pantelides, and M. Scheffler*: Theory of point defects and deep impurities in semiconductors. In: Proc. 11th Int. Conf. on Defects and Radiation Effects in Semiconductors. (Ed.) R.R. Hasiguti. Inst. of Phys., London 1981, 1.

16. *Scheffler, M., S.T. Pantelides, N.O. Lipari, and J. Bernholc*: Identification and properties of native defects in GaP. Phys. Rev. Lett. **47**, 413 (1981).

17. *Berndt, W., R. Hora, and M. Scheffler*: A LEED analysis of c(2x2) sulphur on Pd(100). Surf. Sci. **117**, 188 (1982).

18. *Bernholc, J., N.O. Lipari, S.T. Pantelides, and M. Scheffler*: Electronic structure of deep *sp*-bonded impurities in silicon. Phys. Rev. B **26**, 5706 (1982).

19. *Scheffler, M.*: Electronic structure of simple deep-level defects in semiconductors. Festkörperprobleme **XXII**. (Ed.) P. Grosse. Vieweg, Braunschweig 1982, 115.

20. *Scheffler, M., J.P. Vigneron, and G.B. Bachelet*: Tractable approach for calculating lattice distortions around simple defects in semiconductors: Application to the single donor Ge in GaP. Phys. Rev. Lett. **49**, 1765 (1982).

21. *Schirmer, O. and M. Scheffler*: Determination of deep donor binding energies from their g values. J. Phys. C: Solid State Physics **15**, L645 (1982).

22. *Pantelides, S.T., I. Ivanov, M. Scheffler, and J.P. Vigneron*: Multivacancies, interstitials, and self-interstitial migration in Si. Physica B **116**, 18 (1983).

23. *Scheffler, M. and A.M. Bradshaw*: The electronic structure of adsorbed layers. In: The Chemical Physics of Solid Surfaces and Heterogeneous Catalysis, Vol. 2: Adsorption at Solid Surfaces. (Eds.) D.A. King and D.P. Woodruff. Elsevier, Amsterdam 1983, 165.

24. *Vigneron, J.P., M. Scheffler, and S.T. Pantelides*: Electronic structure of self-interstitials and *sp*-bonded interstitial impurities in semiconductors. Physica B/C **117/118**, 137 (1983).

25. *Hora, R. and M. Scheffler*: Angle-resolved photoemission and the electronic structure of Pd(111). Phys. Rev. B **29**, 692 (1984).

26. *Meyer, B.K., J.-M. Spaeth, and M. Scheffler*: Optical properties of As antisite and EL2 defects in GaAs. Phys. Rev. Lett. **52**, 851 (1984).

27. Scheffler, M., J. Bernholc, N.O. Lipari, and S.T. Pantelides: Electronic structure an identification of deep defects in GaP. Phys. Rev. B **29**, 3269 (1984).
28. Schweitzer, L. and M. Scheffler: Electronic properties of strained bonds in amorphous silicon: The origin of the band-tail states. In: Proc. Optical Effects in Amorphous Semiconductors, Snowbird, Utah, August 1984, American Institute of Physics 1984, 379.

29. Bachelet, G.B. and M. Scheffler: No large lattice relaxations around the arsenic antisite in GaAs. In: Proc. 17th Int. Conf. on the Physics of Semiconductors. (Eds.) J.D. Chadi and W.A. Harrison. Springer New York 1985, 755.
30. Beeler, F., O.K. Andersen, and M. Scheffler: Electronic structure calculation of 3d-transition metal point defects in silicon. In: Microscopic Identification of Electronic Defects in Semiconductors. (Eds.) N.M. Johnson, S.G. Bishop, and G.D. Watkins. MRS, Pittsburgh, Pennsylvania 1985, 129.
31. Beeler, F., O.K. Andersen, and M. Scheffler: Theoretical evidence for low-spin ground states of early interstitial and late substitutional 3d transition-metal ions in silicon. Phys. Rev. Lett. **55**, 1498 (1985).
32. Beeler, F., M. Scheffler, O. Jepsen, and O. Gunnarsson: Identification of chalcogen defects in silicon. In: Microscopic Identification of Electronic Defects in Semiconductors. (Eds.) N.M. Johnson, S.G. Bishop, and G.D. Watkins. MRS, Pittsburgh, Pennsylvania 1985, 117.
33. Beeler, F., M. Scheffler, O. Jepsen, and O. Gunnarsson: Identification of chalcogen point-defect sites in silicon by total-energy calculations. Phys. Rev. Lett. **54**, 2525 (1985).
34. Máca, F. and M. Scheffler: Calculation of the Green's function for a crystal surface or interface. Comput. Phys. Commun. **38**, 403 (1985).
35. Máca, F., M. Scheffler, and W. Berndt: A LEED analysis of $(\sqrt{3} \times \sqrt{3})$ S on Pd(111). In: Proc. 3rd Symposium on Surface Physics: Physics of Solid Surfaces. (Ed.) J. Koukal. Elsevier, Amsterdam 1985, 195.
36. Máca, F., M. Scheffler, and W. Berndt: The adsorption of sulphur on Pd(111). Part I: A LEED analysis of the $(\sqrt{2} \times \sqrt{3})$ R 30° adsorbate structure. Surf. Sci. **160**, 467 (1985).
37. Meyer, B.K., J.-M. Spaeth, and M. Scheffler: As_{Ga}-induced dichroism in GaAs. Respond. Phys. Rev. Lett. **54**, 1333 (1985).
38. Scheffler, M., F. Beeler, O. Jepsen, O. Gunnarsson, O.K. Andersen, and G.B. Bachelet: Chemical bonding and lattice relaxations of deep-level defects. J. of Electronic Materials **14a**, 45 (1985).
39. Scheffler, M., J.P. Vigneron, and G.B. Bachelet: Total- energy gradients and lattice distortions at point defects in semiconductors. Phys. Rev. B **31**, 6541 (1985).

40. *Scheffler, M. and U. Scherz*: Resonant Raman scattering at point defects in GaAs. In: Defects in Semiconductors. (Ed.) H.J. von Bardeleben. Trans Tech Publications Ltd., Switzerland, Mat. Sci. Forum **10-12**, 353 (1986).
41. *Weinert, C.M. and M. Scheffler*: Chalcogen and vacancy pairs in silicon: Electronic structure and stabilities. In: Defects in Semiconductors. (Ed.) H.J. von Bardeleben. Trans Tech Publications Ltd., Switzerland, Mat. Sci. Forum **10-12**, 25 (1986).
42. *Beeler, F., O.K. Andersen, and M. Scheffler*: Electronic structure calculation of 3d and 4d transition metal point defects in silicon. In: Proc. 18th Int. Conf. on the Physics of Semiconductors. (Ed.) O. Engstroem. World Scientific, Singapore 1987, 875.
43. *Beeler, F., O. Jepsen, O.K. Andersen, O. Gunnarsson, and M. Scheffler*: Electronic structure calculation of point defects in silicon. Comput. Phys. Comm. **44**, 297 (1987).
44. *Máca, F. and M. Scheffler*: A new version of the program for the calculation of the Green's function for a crystal surface or interface. Comput. Phys. Comm. **47**, 349 (1987).
45. *Scheffler, M.*: Lattice relaxations at substitutional impurities in semiconductors. Physica B/C **146**, 176 (1987).
46. *Scheffler, M., F. Beeler, O.K. Andersen., O. Gunnarsson, and O. Jepsen*: Parameter-free total-energy and force calculations for defects in semiconductors. In: Proc. 7th Int. School Defects in Crystals. (Ed.) E. Mizera. World Scientific, Singapore 1987, 3.
47. *Weinert, C.M. and M. Scheffler*: Mechanisms of defect pairing in semiconductors: A study for chalcogens in silicon. Phys. Rev. Lett. **58**, 1456 (1987).
48. *Dabrowski, J. and M. Scheffler*: Ab-initio calculations for native point defects in GaAs. In: Proc. 5th Conf. on Semi-Insulating III-V Materials. (Eds.) G. Grossmann, L. Ledebro. Hilger, Bristol 1988, 37.
49. *Dabrowski, J. and M. Scheffler*: The EL2 defect in GaAs. In: Proc. 8th Int. School on Defects in Crystals. (Ed.) E. Mizera. World Scientific, Singapore 1988, 425.
50. *Dabrowski, J. and M. Scheffler*: Theoretical evidence for an optically inducible structural transition of the isolated As antisite in GaAs: Identification and explanation of EL2. Phys. Rev. Lett. **60**, 2183 (1988).
51. *Máca, F. and M. Scheffler*: Calculation of electronic structure for a crystal surface or interface. In: Proc. 4th Symposium on Surface Physics. (Ed.) J. Koukal. Elsevier Sci. Publ., Amsterdam 1988, 221.

52. *Máca, F. and M. Scheffler*: Surface Green's function for a rumpled crystal surface. *Comput. Phys. Commun.* **51**, 381 (1988).
53. *Said, M., F. Máca, K. Kambe, M. Scheffler, and N.E. Christensen*: Electronic structure of fcc and bcc close-packed silver surfaces. *Phys. Rev. B* **38**, 8505 (1988).
54. *Scheffler, M.*: Thermodynamic aspects of bulk and surface defects – first-principle calculations –. In: *Physics of Solid Surfaces 1987*. (Ed.) J. Koukal. Elsevier, Amsterdam 1988, 115.
55. *Scheffler, M. and J. Dąbrowski*: Parameter-free calculations of total energies, interatomic forces and vibrational entropies of defects in semiconductors. *Phil. Mag. A* **58**, 107 (1988).
56. *Weinert, C.M., F. Beeler, and M. Scheffler*: Total-energy calculation for isolated oxygen impurities in silicon. *J. Phys. C* **21**, 841 (1988).

57. *Beeler, F. and M. Scheffler*: Calculation of total energies, reaction and diffusion processes of transition-metal point defects in silicon. In: *Proc. Int. Conf. on the Physics of Semiconductors (ICPS-19)*. (Ed.) W. Zawadzki. Institute of Physics of the Polish Academy of Sciences, Wrocław 1989, 983.
58. *Beeler, F. and M. Scheffler*: Theory of 4d-transition-metal ions in silicon: Total-energies, diffusion, electronic and magnetic properties. *Mat. Sci. Forum* **38-41**, 257 (1989).
59. *Biernacki, S. and M. Scheffler*: Negative thermal expansion of diamond and zinc-blende semiconductors. *Phys. Rev. Lett.* **63**, 290 (1989).
60. *Biernacki, S., U. Scherz, R. Gillert, and M. Scheffler*: Calculated thermodynamic potentials for the vacancy and the oxygen a-center in silicon. *Mat. Sci. Forum* **38-41**, 625 (1989).
61. *Dąbrowski, J. and M. Scheffler*: The As_{Ga}-As_i pair in GaAs, the arsenic antisite and the properties of EL2. In: *Proc. Int. Conf. on the Physics of Semiconductors (ICPS-19)*. (Ed.) W. Zawadzki. Institute of Physics of the Polish Academy of Sciences, Wrocław 1989, 1023.
62. *Dąbrowski, J. and M. Scheffler*: The EL2 defect in GaAs. *Mat. Sci. Forum* **38-41**, 51 (1989).
63. *Dąbrowski, J. and M. Scheffler*: The isolated arsenic antisite defect in GaAs and the properties of EL2. *Phys. Rev. B* **40**, 10391 (1989).
64. *Overhof, H., M. Scheffler, and C.M. Weinert*: *Ab initio* calculations of hyperfine fields for chalcogen point defects and defect pairs in silicon: Identification of the pair atomic structure. *Mater. Sci. Engin. B* **4**, 315 (1989).
65. *Overhof, H., M. Scheffler, and C.M. Weinert*: Computation of hyperfine interactions for substitutional Se⁺ and S⁺ impurities in silicon. *Mat. Sci. Forum* **38-41**, 293 (1989).

66. Scheffler, M.: Chemical binding, stability and metastability of defects in semiconductors. Festkörperprobleme **29**. (Ed.) U. Rössler. Vieweg, Braunschweig 1989, 231.
67. Scherz, U., D. Weider, and M. Scheffler: Electronic and vibrational properties of deep centers in semiconductors. Egyp. J. Sol. **12**, 1 (1989).
68. Weider, D., M. Scheffler, and U. Scherz: Parameter-free calculations of the pressure dependence of impurity levels, entropies and of defect-formation volumes. Mat. Sci. Forum **38-41**, 299 (1989).

69. Beeler, F., O.K. Andersen, and M. Scheffler: Electronic and magnetic structure of 3d-transition-metal point defects in silicon calculated from first principles. Phys. Rev. B **41**, 1603 (1990).
70. Biernacki, S. and M. Scheffler: First-principles calculations of thermodynamic potentials of perfect-crystal semiconductors and for defects in semiconductors. In: Proc. 4th Brazilian School of Semiconductor Physics. (Eds.) A.S. Chaves, A.G. de Oliveira, and C.E.T. Gonzalves da Silva. World Scientific, Singapore 1990, 188.
71. Caldas, M.J., J. Dąbrowski, A. Fazzio, and M. Scheffler: Anion antisite-like defects in III-V compounds. In: Proc. Int. Conf. on the Physics of Semiconductors (ICPS-20). (Eds.) E.M. Anastassakis, J.D. Joannopoulos. World Scientific, Singapore 1990, 469.
72. Caldas, M.J., J. Dąbrowski, A. Fazzio, and M. Scheffler: Anion antisite-like defects in III-V compounds. Phys. Rev. Lett. **65**, 2046 (1990).
73. Caldas, M.J., A. Fazzio, J. Dąbrowski, and M. Scheffler: Anion-antisite defects in GaAs: As and Sb. In: International Journal of Quantum Chemistry: Quantum Chemistry Symposium 24, 563 (1990).
74. Dąbrowski, J., M. Scheffler, and R. Strehlow: Silicon donor in gallium arsenide and its relation to DX centers. In: Proc. Int. Conf. on the Physics of Semiconductors (ICPS-20). (Eds.) E.M. Anastassakis, J.D. Joannopoulos. World Scientific, Singapore 1990, 489.
75. Doyen, G., E. Koetter, J.P. Vigneron, and M. Scheffler: Theory of scanning tunneling microscopy. Appl. Phys. A **51**, 281 (1990).
76. Gonze, X., P. Käckell, and M. Scheffler: Ghost states for separable, norm-conserving, ab-initio pseudopotentials. Phys. Rev. B **41**, 12264 (1990).
77. Hebenstreit, J., M. Heinemann, and M. Scheffler: Calculated surface geometries and electronic structures for clean and sodium covered GaAs (110) surfaces. In: Electronic, Optical and Device Properties of Layered Structures. (Eds.) J.R. Hayes, M.S. Hybertsen, and E.R. Weber. MRS, Pittsburgh 1990, 71.

78. *Hebenstreit, J., M. Heinemann, and M. Scheffler*: Calculated surface geometries, photothresholds, and Schottky-barrier heights for alkalis adsorbed on GaAs(110). In: Proc. Int. Conf. on the Physics of Semiconductors (ICPS-20). (Eds.) E.M. Anastassakis, J.D. Joannopoulos. World Scientific, Singapore 1990, 215.
79. *Máca, F., M. Said, K. Kambe, and M. Scheffler*: Electronic structure and angular resolved photoemission calculations for fcc and bcc silver surfaces. Vacuum **41**, 538 (1990).
80. *Methfessel, M., B.K. Agrawal, and M. Scheffler*: The influence of structural relaxation on the valence-band offset at semiconductor-semiconductor interfaces. In: Proc. Int. Conf. on the Physics of Semiconductors (ICPS-20). (Eds.) E.M. Anastassakis, J.D. Joannopoulos. World Scientific, Singapore 1990, 989.
81. *Vigneron, J.P., M. Scheffler, Th. Laloyaux, I. Derycke, and A. Lucas*: Spatial electron current distribution in a scanning tunneling microscope. Vacuum **41**, 745 (1990).
82. *Alves, J.L.A., J. Hebenstreit, and M. Scheffler*: Calculated atomic structures and electronic properties of GaP, InP, GaAs and InAs (110) surfaces. Phys. Rev. B **44**, 6188 (1991).
83. *Gonze, X., R. Stumpf, and M. Scheffler*: Analysis of fully separable potentials. Phys. Rev. B **44**, 8503 (1991).
84. *Hebenstreit, J., M. Heinemann, and M. Scheffler*: Atomic and electronic structures of GaAs (110) and their alkali-adsorption induced changes. Phys. Rev. Lett. **67**, 1031 (1991).
85. *Methfessel, M., D. Hennig, S. Weber, and M. Scheffler*: Ab-initio calculation of the effect of *d*-band occupation on the relaxation of transition metal surfaces. Proc. 75th WE-Heraeus-Seminar and 21st Annual Internat. Symposium on Electronic Structure of Solids. (Eds.) P. Ziesche, H. Eschrig. Akademie Verlag, Berlin 1991, 174.
86. *Methfessel, M. and M. Scheffler*: Full-potential LMTO calculations for atomic relaxations at semiconductor-semiconductor interfaces. Physica B **172**, 175 (1991).
87. *Overhof, H., M. Scheffler, and C.M. Weinert*: Formation energies, electronic structure, and hyperfine fields of chalcogen point defects and defect pairs in silicon. Phys. Rev. B **43**, 12494 (1991).
88. *Scheffler, M., Ch. Droste, A. Fleszar, F. Máca, G. Wachutka, and G. Barzel*: A self-consistent surface-Green-function (SSGF) method. Physica B **172**, 143 (1991).
89. *Schmalz, A., S. Aminpirooz, L. Becker, J. Haase, J. Neugebauer, M. Scheffler, D.R. Batchelor, D.L. Adams, and E. Bøgh*: Unusual chemisorption geometry of Na on Al (111). Phys. Rev. Lett. **67**, 2163 (1991).

90. *Dąbrowski, J., E. Pehlke, and M. Scheffler*: DFT-LDA calculations of surface core-level shifts for Si(001), Ge(001), and Ge on Si(001) (2×1) surfaces. In: Proc. 21st Int. Conf. on the Physics of Semiconductors. (Eds.) P. Jiang, H.Z. Zheng. World Scientific, Singapore 1992, 389.
91. *Dąbrowski, J. and M. Scheffler*: Defect metastability in III-V compounds. *Mat. Sci. Forum* **83-87**, 735 (1992).
92. *Dąbrowski, J. and M. Scheffler*: Self-consistent study of the electronic and structural properties of the clean Si (001) (2x1) surface. *Appl. Surf. Sci.* **56-58**, 15 (1992).
93. *Dąbrowski, J. and M. Scheffler*: Theory of defect metastabilities in III-V compounds. *Physica Scripta* **T45**, 151 (1992).
94. *Doyen, G., D. Drakova, V. Mujica, and M. Scheffler*: Theory of the scanning tunneling microscope. *Phys. Stat. Sol. (a)* **131**, 107 (1992).
95. *Hebenstreit, J. and M. Scheffler*: Self-consistent pseudopotential calculations for sodium adsorption on GaAs(110). *Phys. Rev. B* **46**, 10134 (1992).
96. *Heinemann, M. and M. Scheffler*: Formation energies and abundances of intrinsic point defects at the GaAs/AlAs (100) interface. *Appl. Surf. Sci.* **56-58**, 628 (1992).
97. *Methfessel, M., D. Hennig, and M. Scheffler*: Trends of the surface relaxations, surface energies, and work functions of the 4d transition metals. *Phys. Rev. B* **46**, 4816 (1992).
98. *Methfessel, M., D. Hennig, and M. Scheffler*: Calculated surface energies of the 4d transition metals: A study of bond-cutting models. *Appl. Phys. A* **55**, 442 (1992).
99. *Neugebauer, J. and M. Scheffler*: Adsorbate-substrate and adsorbate-adsorbate interactions of Na and K adlayers on Al(111). *Phys. Rev. B* **46**, 16067 (1992).
100. *Ourmazd, A., M. Scheffler, M. Heinemann, and J.-L. Rouviere*: Microscopic properties of thin films: Learning about point defects. MRS Bulletin “Quantitative Analysis of Thin Films”, Part I, **XVII**, No. 12, 24 (1992).
101. *Stampfl, C., M. Scheffler, H. Over, J. Burchhardt, M. Nielsen, D. Adams, and W. Moritz*: Identification of stable and metastable adsorption sites for K adsorbed on Al(111). *Phys. Rev. Lett.* **69**, 1532 (1992).
102. *Wachutka, G., A. Fleszar, F. Máca, and M. Scheffler*: Self-consistent Green-function method for the calculation of electronic properties of localized defects at surfaces and in the bulk. *J. Phys. C* **4**, 2831 (1992).
103. *Aristov, V. Yu., M. Bertolo, K. Jacobi, F. Máca, and M. Scheffler*: Experimental and theoretical investigation of the electronic structure of silver deposited onto InSb (110) at 10 K. *Phys. Rev. B* **48**, 5555 (1993).

104. *Bechstedt, F. and M. Scheffler*: Alkali adsorption on GaAs (110): atomic structure, electronic states and surface dipoles. *Surf. Sci. Reports* **18**, 145 (1993).
105. *Doyen, G., D. Drakova, and M. Scheffler*: Green-function theory of scanning tunneling microscopy: Tunnel current and current density for clean metal surfaces. *Phys. Rev. B* **47**, 9778 (1993).
106. *Fiorentini, V., M. Methfessel, and M. Scheffler*: Electronic and structural properties of GaN by the full-potential linear muffin-tin orbitals method: The role of the *d* electrons. *Phys. Rev. B* **47**, 13353 (1993).
107. *Fiorentini, V., M. Methfessel, and M. Scheffler*: Reconstruction mechanism of fcc transition metal (001) surfaces. *Phys. Rev. Lett.* **71**, 1051 (1993); *Phys. Rev. Lett.* **81**, 2184(E) (1998).
108. *Hennig, D., M. Methfessel, and M. Scheffler*: Ab-initio calculations of the initial- and final-state effects on core-level shifts at transition metal surfaces. In: Proc. ICPTM. (Eds.) P.M. Oppeneer, J. Kübler. World Scientific, Singapore 1993, 542.
109. *Kraft, T., P.M. Marcus, M. Methfessel, and M. Scheffler*: Elastic constants of Cu and the instability of its bcc structure. *Phys. Rev. B* **48**, 5886 (1993).
110. *Kraft, T., M. Methfessel, M. van Schilfgaarde, and M. Scheffler*: Effect of substrate-imposed strain on the growth of metallic overlayers calculated for fcc and hcp iron. *Phys. Rev. B* **47**, 9862 (1993).
111. *Kraft, T., M. Methfessel, M. van Schilfgaarde, and M. Scheffler*: Elastic properties of strained fcc and hcp iron. In: Proc. ICPTM. (Eds.) P.M. Oppeneer, J. Kübler. World Scientific, Singapore 1993, 207.
112. *Methfessel, M., D. Hennig, and M. Scheffler*: Ab-initio calculations of the initial- and final-state effects on the surface core-level shift of transition metals. *Surf. Sci.* **287/288**, 785 (1993).
113. *Methfessel, M., M. van Schilfgaarde, and M. Scheffler*: Electronic structure and bonding in the metallocarbohedrene Ti_8C_{12} . *Phys. Rev. Lett.* **70**, 29 (1993); **71**, 209(E) (1993).
114. *Neugebauer, J. and M. Scheffler*: Mechanisms of island formation of alkali-metal adsorbates on Al(111). *Phys. Rev. Lett.* **71**, 577 (1993).
115. *Neugebauer, J. and M. Scheffler*: Theory of adsorption and desorption in high electric fields. *Surf. Sci.* **287/288**, 572-576 (1993).
116. *Oppo, S., V. Fiorentini, and M. Scheffler*: Theory of adsorption and surfactant effect of Sb on Ag(111). *Phys. Rev. Lett.* **71**, 2437 (1993).
117. *Pankratov, O. and M. Scheffler*: Bound bipolaron at the surface: The negative-*U* behavior of GaAs (110) with adsorbed alkali metals. *Phys. Rev. Lett.* **71**, 2797 (1993).

118. *Pankratov, O. and M. Scheffler*: Clustering and correlations on GaAs-metal interface. In: Semiconductor Interfaces at the Sub-Nanometer Scale. (Eds.) H.W.M. Salemink, M.D. Pashley. NATO ASI Series E: Applied Sciences **243**, Kluwer Academic Publishers, The Netherlands 1993, 121.
119. *Pankratov, O. and M. Scheffler*: Electron correlations on potassium-covered GaAs (110) surface: ab-initio calculations of the Hubbard U . *Surf. Sci.* **287/288**, 584 (1993).
120. *Pankratov, O. and M. Scheffler*: Hubbard correlations and charge transfer at the GaAs (110) surface with alkali adsorbates. *Phys. Rev. Lett.* **70**, 351 (1993).
121. *Pehlke, E. and M. Scheffler*: Evidence for site-sensitive screening of core holes at the Si and Ge (001) surface. *Phys. Rev. Lett.* **71**, 2338 (1993).
122. *Polatoglou, H.M., M. Methfessel, and M. Scheffler*: Vacancy-formation energies at the (111) surface and in bulk Al, Cu, Ag, and Rh. *Phys. Rev. B* **48**, 1877 (1993).
123. *Scheffler, M., J. Neugebauer, and R. Stumpf*: A step from surface fiction towards surface science. *J. Phys.: Condens. Matter* **5**, A91 (1993).
124. *Scherz, U. and M. Scheffler*: Density-functional theory of *sp*-bonded defects in III-V semiconductors. In: Semiconductors and Semimetals, Vol. 38 (Imperfections in III/V Materials). (Ed.) E. Weber. Academic Press, Boston 1993, 1.
125. *Stampfl, C., J. Burchhardt, M. Nielsen, D.L. Adams, M. Scheffler, H. Over, and W. Moritz*: The structure of Al(111)-K-($\sqrt{3} \times \sqrt{3}$)R30° determined by LEED: stable and metastable adsorption sites. *Surf. Sci.* **287/288**, 418 (1993).
126. *Wenzien, B., J. Bormet, J. Neugebauer, and M. Scheffler*: Electronic structure of ($\sqrt{3} \times \sqrt{3}$) - R30° Na and K on Al(111): Comparison of “normal” and substitutional adsorption sites. *Surf. Sci.* **287/288**, 559 (1993).
127. *Ziegler, Ch., U. Scherz, and M. Scheffler*: Pressure dependence of deep levels of the As-antisite, the Ga-vacancy-As-interstitial pair, and of the stable and metastable states of *EL2*. *Phys. Rev. B* **47**, 16624 (1993).

128. *Andersen, J.N., D. Hennig, E. Lundgren, M. Methfessel, R. Nyholm, and M. Scheffler*: Surface core-level shifts of some 4d-metal single-crystal surfaces: Experiments and *ab initio* calculations. *Phys. Rev. B* **50**, 17525 (1994).
129. *Biernacki, S. and M. Scheffler*: The influence of the isotopic composition on the thermal expansion of crystalline Si. *J. Phys.: Condens. Matter* **6**, 4879 (1994).
130. *Bormet, J., J. Neugebauer, and M. Scheffler*: Chemical trends and bonding mechanisms for isolated adsorbates on Al(111). *Phys. Rev. B* **49**, 17242 (1994).
131. *Bormet, J., B. Wenzien, and M. Scheffler*: A self-consistent surface Green-function (SSGF) method for the calculation of isolated adsorbate atoms on a semi-infinite crystal. *Comput. Phys. Commun.* **79**, 124 (1994).

132. *Dąbrowski, J., E. Pehlke, and M. Scheffler*: Calculation of the surface stress anisotropy for the buckled Si (001)(1×2) and p (2×2) surfaces. *Phys. Rev. B* **49**, 4790 (1994).
133. *Dąbrowski, J., E. Pehlke, and M. Scheffler*: Relation between the atomic structure and the surface-stress anisotropy: Calculations for the clean Si (001) surface. *J. Vac. Sci. Technol. B* **12**, 2675 (1994).
134. *Gross, A., B. Hammer, M. Scheffler, and W. Brenig*: High-dimensional quantum dynamics of adsorption and desorption of H₂ at Cu (111). *Phys. Rev. Lett.* **73**, 3121 (1994).
135. *Hammer, B., M. Scheffler, K.W. Jacobsen, and J.K. Nørskov*: Multidimensional potential energy surface for H₂ dissociation over Cu (111). *Phys. Rev. Lett.* **73**, 1400 (1994).
136. *Heinemann, M. and M. Scheffler*: The formation of a Schottky barrier: Na on GaAs (110). In: Proc. 4th Int. Conf. on the Formation of Semiconductor Interfaces (ICFSI-4). (Eds.) B. Lengeler, H. Lüth, W. Mönch, J. Pollmann. World Scientific, Singapore 1994, 297.
137. *Heinemann, M. and M. Scheffler*: Thick sodium overlayers on GaAs (110). *Phys. Rev. B* **49**, 5516 (1994).
138. *Hennig, D., M. Methfessel, and M. Scheffler*: Ab initio calculation of surface core-level shifts for transition metal surfaces. *Surf. Sci.* **307-309**, 933 (1994).
139. *Kohler, B., M. Fuchs, K. Freihube, and M. Scheffler*: Comment on “Local exchange-correlation functional: Numerical test for atoms and ions”. *Phys. Rev. A* **49**, 5152 (1994).
140. *Kraft, T., P.M. Marcus, and M. Scheffler*: Atomic and magnetic structure of fcc Fe/Cu (100). *Phys. Rev. B* **49**, 11511 (1994).
141. *Neugebauer, J. and M. Scheffler*: Alkali-metal adsorbates on aluminum (111): The interplay and competition of adsorbate-substrate and adsorbate-adsorbate interactions. *Prog. Surf. Sci.* **46**, 295 (1994).
142. *Oppo, S., V. Fiorentini, and M. Scheffler*: Surface alloying and surfactant action of Sb on Ag (111). *Mat. Res. Soc. Symp. Proc.* **317**, 323 (1994).
143. *Pankratov, O. and M. Scheffler*: Surface polarons and bipolarons at GaAs (110) with adsorbed alkali metals. *Surf. Sci.* **307-309**, 1001 (1994).
144. *Stampfl, C., J. Neugebauer, and M. Scheffler*: Alkali-metal adsorption on Al (111) and Al (100). *Surf. Sci.* **307-309**, 8 (1994).
145. *Stampfl, C., J. Neugebauer, and M. Scheffler*: Theoretical evidence for unusual bonding geometry and phase transitions of Na on Al (001). *Surf. Rev. Lett.* **1**, 213 (1994).
146. *Stampfl, C. and M. Scheffler*: Theoretical identification of a (2×2) composite double layer ordered surface alloy of Na on Al (111). *Surf. Sci.* **319**, L23 (1994).

147. *Stampfl, C., M. Scheffler, H. Over, J. Burchhardt, M. Nielsen, D. L. Adams, and W. Moritz*: A LEED structural analysis of Al(111)-K-($\sqrt{3} \times \sqrt{3}$)R30°: Identification of stable and metastable adsorption sites. *Phys. Rev. B* **49**, 4959 (1994).
148. *Stumpf, R. and M. Scheffler*: Mechanisms of self-diffusion on flat and stepped Al surfaces. *Surf. Sci.* **307-309**, 501 (1994).
149. *Stumpf, R. and M. Scheffler*: Simultaneous calculation of the equilibrium atomic structure and its electronic ground state using density-functional theory. *Comput. Phys. Commun.* **79**, 447 (1994).
150. *Stumpf, R. and M. Scheffler*: Theory of self-diffusion at and growth of Al(111). *Phys. Rev. Lett.* **72**, 254-257 (1994); **73**, 508 (1994).
151. *Wilke, S., D. Hennig, R. Löber, M. Methfessel, and M. Scheffler*: *Ab initio* study of hydrogen adsorption on Pd(100). *Surf. Sci.* **307-309**, 76 (1994).
152. *Yamada, K., T. Kraft, T. Aisaka, A. Ishii, and M. Scheffler*: Spin- and angle-resolved UPS spectrum calculation for ferromagnetic Nickel. *Trans. Mat. Res. Soc. Jpn.*, **16A**, 259 (1994).
153. *Ziegler, Ch., U. Scherz, and M. Scheffler*: Pressure dependences of transition energies of the As antisite and the Ga-vacancy-As-interstitial pair compared to stable and metastable EL2. *Mat. Sci. Forum* **143-147**, 995 (1994).
154. *Becker, P., U. Kütgens, J. Stumpel, S. Biernacki, and M. Scheffler*: The silicon-28 lattice parameter. *PTB-Mitteilungen* **105**, 95 (1995).
155. *Berndt, W., D. Weick, C. Stampfl, A.M. Bradshaw, and M. Scheffler*: Structural analysis of the two c(2×2) phases of Na adsorbed on Al(100). *Surf. Sci.* **330**, 182 (1995).
156. *Burchhardt, J., M.M. Nielsen, D.L. Adams, E. Lundgren, J.N. Andersen, C. Stampfl, M. Scheffler, A. Schmalz, S. Aminpirooz, and J. Haase*: Formation and structural analysis of a surface alloy: Al(111)-(2×2)-Na. *Phys. Rev. Lett.* **74**, 1617 (1995).
157. *Finnis, M.W., R. Kaschner, C. Kruse, J. Furthmüller, and M. Scheffler*: The interaction of a point charge with a metal surface: theory and calculations for (111), (100) and (110) aluminium surfaces. *J. Phys.: Condens. Matter* **7**, 2001 (1995).
158. *Fiorentini, V., M. Methfessel, and M. Scheffler*: Surface stress, relaxation and reconstruction in fcc transition metals. *Vuoto* **XXIV**, 21 (1995).
159. *Fiorentini, V., S. Oppo, and M. Scheffler*: Towards an understanding of surfactant action on the epitaxial growth of metals: The case of Sb on Ag(111). *Appl. Phys. A* **60**, 399 (1995).
160. *Furthmüller, J., G. Kresse, J. Hafner, R. Stumpf, and M. Scheffler*: Site-selective adsorption of C atoms on Al(111) surfaces. *Phys. Rev. Lett.* **74**, 5084 (1995).

161. Gross, A., S. Wilke, and M. Scheffler: Six-dimensional quantum dynamics of adsorption and desorption of H₂ at Pd(100): Steering and steric effects. Phys. Rev. Lett. **75**, 2718 (1995).
162. Hammer, B. and M. Scheffler: Local chemical reactivity of a metal alloy surface. Phys. Rev. Lett. **74**, 3487 (1995).
163. Hanbicki, A.T., A.P. Baddorf, E.W. Plummer, B. Hammer, and M. Scheffler: The interaction of hydrogen with the (110) surface of NiAl. Surf. Sci. **333**, 811 (1995).
164. Kley, A., J. Neugebauer, and M. Scheffler: Interface stability and valence-band offsets for the GaAs/ZnSe(001) heterojunction. In: Proc. 22nd Int. Conf. on the Physics of Semiconductors. (Ed.) D.J. Lockwood. World Scientific, Singapore 1995, 775.
165. Kohler, B., P. Ruggerone, S. Wilke, and M. Scheffler: Frustrated H-induced instability of Mo(110). Phys. Rev. Lett. **74**, 1387 (1995).
166. Methfessel, M., D. Hennig, and M. Scheffler: Enhanced screening of core holes at transition-metal surfaces. Surf. Rev. Lett. **2**, 197 (1995).
167. Moll, N., M. Bockstedte, M. Fuchs, E. Pehlke, and M. Scheffler: Application of generalized gradient approximations: the diamond- β -tin phase transition in Si and Ge. Phys. Rev. B **52**, 2550 (1995).
168. Oppo, S., V. Fiorentini, and M. Scheffler: Size-effect surfactants for metal-on-metal growth: Sb on Ag(111). Vuoto **XXIV**, 37 (1995).
169. Pankratov, O. and M. Scheffler: Formation of localized excitons and the breaking of chemical bonds at III-V (110) surfaces. In: Proc. 22nd Int. Conf. on the Physics of Semiconductors. (Ed.) D.J. Lockwood. World Scientific, Singapore 1995, 485.
170. Pankratov, O. and M. Scheffler: Localized excitons and breaking of chemical bonds at III-V (110) surfaces. Phys. Rev. Lett. **75**, 701 (1995).
171. Pehlke, E. and M. Scheffler: Hydrogen adsorption on and desorption from Si(001). In: Proc. 22nd Int. Conf. on the Physics of Semiconductors. (Ed.) D.J. Lockwood. World Scientific, Singapore 1995, 549.
172. Pehlke, E. and M. Scheffler: Theory of adsorption and desorption of H₂/Si(001). Phys. Rev. Lett. **74**, 952 (1995).
173. Ruggerone, P., B. Kohler, S. Wilke, and M. Scheffler: Electronic origin of the H-induced phonon anomalies on Mo(110). In: Electronic Surface and Interface States on Metallic Systems. (Eds.) E. Bertel, M. Donath. World Scientific, Singapore 1995, 113.
174. Stampfl, C. and M. Scheffler: Theory of alkali-metal adsorption on close-packed metal surfaces. Surf. Rev. Lett. **2**, 317 (1995).
175. Wenzien, B., J. Bormet, and M. Scheffler: Green function for crystal surfaces I. Comput. Phys. Commun. **88**, 230 (1995).

176. *Wilke, S. and M. Scheffler*: Poisoning of Pd(100) for the dissociation of H₂: a theoretical study of co-adsorption of hydrogen and sulfur. *Surf. Sci.* **329**, L605 (1995).
177. *Cho, J.-H. and M. Scheffler*: *Ab initio* pseudopotential study of Fe, Co, and Ni employing the spin-polarized LAPW approach. *Phys. Rev. B* **53**, 10685 (1996).
178. *Gross, A., M. Bockstedte, and M. Scheffler*: *Ab initio* molecular dynamics study of D₂ desorption from Si(100). In: Proc. 23rd Int. Conf. on the Physics of Semiconductors. (Eds.) M. Scheffler, R. Zimmermann. World Scientific, Singapore 1996, 951.
179. *Gross, A. and M. Scheffler*: Influence of molecular vibrations on dissociative adsorption. *Chem. Phys. Lett.* **256**, 417 (1996).
180. *Gross, A. and M. Scheffler*: Gross and Scheffler Reply. *Phys. Rev. Lett.* **77**, 405 (1996).
181. *Gross, A. and M. Scheffler*: Scattering of hydrogen molecules from a reactive surface: strong off-specular and rotationally inelastic diffraction. *Chem. Phys. Lett.* **263**, 567 (1996).
182. *Gross, A., S. Wilke, and M. Scheffler*: Six-dimensional quantum dynamics of adsorption and desorption of H₂ at Pd(100): no need for a molecular precursor adsorption state. *Surf. Sci.* **357-358**, 614 (1996).
183. *Hennig, D., M.V. Ganduglia-Pirovano, and M. Scheffler*: Adlayer core-level shifts of admetal monolayers on transition-metal substrates and their relation to the surface chemical reactivity. *Phys. Rev. B* **53**, 10344 (1996).
184. *Kley, A. and M. Scheffler*: Diffusivity of Ga and Al adatoms on GaAs(001). In: Proc. 23rd Int. Conf. on the Physics of Semiconductors. (Eds.) M. Scheffler, R. Zimmermann. World Scientific, Singapore 1996, 1031.
185. *Kohler, B., P. Ruggerone, and M. Scheffler*: Anomalies in He atom scattering spectra of the H-covered Mo(110) and W(110) surfaces. *Surf. Sci.* **368**, 213 (1996).
186. *Kohler, B., P. Ruggerone, M. Scheffler, and E. Tosatti*: Enhanced electron-phonon coupling at the Mo and W(110) surfaces induced by adsorbed hydrogen. *Z. Phys. Chemie* **197**, 193 (1996).
187. *Kohler, B., S. Wilke, M. Scheffler, R. Kouba, and C. Ambrosch-Draxl*: Force calculation and atomic-structure optimization for the full-potential linearized augmented plane-wave code WIEN. *Comput. Phys. Commun.* **94**, 31 (1996).
188. *Moll, N., A. Kley, E. Pehlke, and M. Scheffler*: GaAs equilibrium crystal shape from first principles. *Phys. Rev. B* **54**, 8844 (1996).
189. *Pehlke, E., N. Moll, and M. Scheffler*: The equilibrium shape of InAs quantum dots grown on a GaAs(001) substrate. In: Proc. 23rd Int. Conf. on the Physics of Semiconductors. (Eds.) M. Scheffler, R. Zimmermann. World Scientific, Singapore 1996, 1301.

190. Petersen, M., S. Wilke, P. Ruggerone, B. Kohler, and M. Scheffler: Scattering of rare-gas atoms at a metal surface: Evidence of anticorrugation of the helium-atom potential energy surface and the surface electron density. *Phys. Rev. Lett.* **76**, 995 (1996).
191. Scheffler, M., V. Fiorentini, and S. Oppo: Homoepitaxial growth of metals and the role of surfactants. In: *Surface Science: Principles and Current Applications*. (Eds.) R.J. MacDonald, E.C. Taglauer, K.R. Wandelt. Springer, Berlin 1996, 219.
192. Scheffler, M. and R. Zimmermann (Eds.): Proc. 23rd Int. Conf. on the Physics of Semiconductors (ICPS-23). World Scientific, Singapore 1996, 4 volumes.
193. Stampfl, C. and M. Scheffler: Theoretical study of O layers on Ru(0001). *Phys. Rev. B* **54**, 2868 (1996).
194. Stampfl, C., S. Schwegmann, H. Over, M. Scheffler, and G. Ertl: Structure and stability of a high-coverage (1×1) oxygen phase on Ru(0001). *Phys. Rev. Lett.* **77**, 3371 (1996).
195. Stumpf, R. and M. Scheffler: *Ab initio* calculations of energies and self-diffusion on flat and stepped surfaces of Al and their implications on crystal growth. *Phys. Rev. B* **53**, 4958 (1996).
196. Wilke, S., M.H. Cohen, and M. Scheffler: Local isoelectronic reactivity of solid surfaces. *Phys. Rev. Lett.* **77**, 1560 (1996).
197. Wilke, S. and M. Scheffler: Mechanism of poisoning the catalytic activity of Pd(100) by sulfur. *Phys. Rev. Lett.* **76**, 3380 (1996).
198. Wilke, S. and M. Scheffler: Potential-energy surface for H₂ dissociation over Pd(100). *Phys. Rev. B* **53**, 4926 (1996).
199. Yu, B. D. and M. Scheffler: Anisotropy of growth of the close-packed surfaces of silver. *Phys. Rev. Lett.* **77**, 1095 (1996).
200. Alippi, P., P.M. Marcus, and M. Scheffler: Strained tetragonal states and bain paths in metals. *Phys. Rev. Lett.* **78**, 3892 (1997).
201. Arnold, M., G. Hupfauer, P. Bayer, L. Hammer, K. Heinz, B. Kohler, and M. Scheffler: Hydrogen on W(110): an adsorption structure revisited. *Surf. Sci.* **382**, 288 (1997).
202. Bockstedte, M., A. Kley, J. Neugebauer, and M. Scheffler: Density-functional theory calculations for poly-atomic systems: electronic structure, static and elastic properties and *ab initio* molecular dynamics. *Comput. Phys. Commun.* **107**, 187 (1997).
203. Bockstedte, M. and M. Scheffler: Theory of self-diffusion in GaAs. *Z. Phys. Chem.* **200**, 195 (1997).

204. *Cho, J.-H. and M. Scheffler*: Surface relaxation and ferromagnetism of Rh(001). Phys. Rev. Lett. **78**, 1299 (1997).
205. *Ganduglia-Pirovano, M.V., J. Kudrnovský, and M. Scheffler*: Adlayer core-level shifts of random metal overlayers on transition-metal substrates. Phys. Rev. Lett. **78**, 1807 (1997).
206. *Gross, A., M. Bockstedte, and M. Scheffler*: *Ab initio* molecular dynamics study of the desorption of D₂ from Si(100). Phys. Rev. Lett. **79**, 701 (1997).
207. *Gross, A. and M. Scheffler*: Role of zero-point effects in catalytic reactions involving hydrogen. J. Vac. Sci. Technol. A **15**, 1624 (1997).
208. *Gross, A. and M. Scheffler*: Steering and isotope effects in the dissociative adsorption of H₂/Pd(100). In: Frontiers in Materials Modelling and Design V. (Eds.) V. Kumar, S. Sengupta, B. Raj. Springer Proc. in Physics, Springer, Heidelberg 1997, 285.
209. *Gross, A. and M. Scheffler*: Steering and ro-vibrational effects on dissociative adsorption and associative desorption of H₂/Pd(100). Prog. Surf. Sci. **53**, 187 (1997).
210. *Kley, A., P. Ruggerone, and M. Scheffler*: Novel diffusion mechanism on the GaAs (001) surface: The role of adatom-dimer interaction. Phys. Rev. Lett. **79**, 5278 (1997).
211. *Kohler, B., P. Ruggerone, and M. Scheffler*: *Ab initio* study of the anomalies in the He-atom-scattering spectra of H/Mo(110) and H/W(110). Phys. Rev. B **56**, 13503 (1997).
212. *Narasimhan, S. and M. Scheffler*: A model for the thermal expansion of Ag(111) and other metal surfaces. Z. Phys. Chem. **202**, 253 (1997).
213. *Pehlke, E., N. Moll, A. Kley, and M. Scheffler*: Shape and stability of quantum dots. Appl. Phys. A **65**, 525 (1997).
214. *Pehlke, E., N. Moll, and M. Scheffler*: The equilibrium shape of quantum dots. In: Proc. VI Italian-Swiss Workshop on Advances in Computational Materials Science. (Eds.) V. Fiorentini, F. Meloni. Conf. Proc. **55**, Italian Physical Society, Bologna 1997, 23.
215. *Petersen, M., P. Ruggerone, and M. Scheffler*: He scattering from metal surfaces. In: Proc. VI Italian-Swiss Workshop on Advances in Computational Materials Science. (Eds.) V. Fiorentini, F. Meloni. Conf. Proc. **55**, Italian Physical Society, Bologna 1997, 43.
216. *Ratsch, C., P. Ruggerone, and M. Scheffler*: Density-functional theory of surface diffusion and epitaxial growth of metals. In: Surface Diffusion: Atomistic and Collective Processes. (Ed.) M.C. Tringides. NATO ASI Series B: Physics Vol. 360, Plenum Press, New York 1997, 83.
217. *Ratsch, C., A.P. Seitsonen, and M. Scheffler*: Strain dependence of surface diffusion: Ag on Ag(111) and Pt(111). Phys. Rev. B **55**, 6750 (1997).

218. *Ruggerone, P., A. Kley, and M. Scheffler*: Bridging the length and time scales: from *ab initio* electronic structure calculations to macroscopic proportions. In: HCM Newsletter (Ψ_k Network). (Ed.) Z. Szotek. **21**, 75 (1997).
219. *Ruggerone, P., A. Kley, and M. Scheffler*: Microscopic aspects of homoepitaxial growth. *Progr. Surf. Sci.* **54**, 331 (1997).
220. *Ruggerone, P., A. Kley, and M. Scheffler*: Microscopic processes behind metal homoepitaxy. In: Proc. VI Italian-Swiss Workshop on Advances in Computational Materials Science. (Eds.) V. Fiorentini, F. Meloni. Conf. Proc. **55**, Italian Physical Society, Bologna 1997, 33.
221. *Ruggerone, P., C. Ratsch, and M. Scheffler*: Density-functional theory of epitaxial growth of metals. In: Growth and Properties of Ultrathin Epitaxial Layers. (Eds.) D.A. King, D.P. Woodruff. *The Chemical Physics of Solid Surfaces*, Vol. 8. Elsevier Science, Amsterdam 1997, 490.
222. *Stampfl, C. and M. Scheffler*: Anomalous behavior of Ru for catalytic oxidation: A theoretical study of the catalytic reaction $\text{CO} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}_2$. *Phys. Rev. Lett.* **78**, 1500 (1997).
223. *Stampfl, C. and M. Scheffler*: Mechanism of efficient carbon monoxide oxidation at Ru(0001). *J. Vac. Sci. Technol. A* **15**, 1635 (1997).
224. *Stampfl, C. and M. Scheffler*: Study of CO oxidation over Ru(0001) at high gas pressures. *Surf. Sci.* **377-379**, 808 (1997).
225. *Tománek, D., S. Wilke, and M. Scheffler*: Hydrogen-induced polymorphism of the Pd(110) surface. *Phys. Rev. Lett.* **79**, 1329 (1997).
226. *Yu, B. D. and M. Scheffler*: *Ab initio* study of step formation and self-diffusion on Ag(100). *Phys. Rev. B* **55**, 13916 (1997).
227. *Yu, B. D. and M. Scheffler*: Physical origin of exchange diffusion on fcc(100) metal surfaces. *Phys. Rev. B* **56**, R 15569 (1997).
228. *Boisvert, G., L.J. Lewis, and M. Scheffler*: Island morphology and adatom self-diffusion on Pt(111). *Phys. Rev. B* **57**, 1881 (1998).
229. *Fuchs, M., M. Bockstedte, E. Pehlke, and M. Scheffler*: Pseudopotential study of binding properties of solids within generalized gradient approximations: The role of core-valence exchange-correlation. *Phys. Rev. B* **57**, 2134 (1998).
230. *Gross, A. and M. Scheffler*: *Ab initio* quantum and molecular dynamics of the dissociative adsorption of hydrogen on Pd(100). *Phys. Rev. B* **57**, 2493 (1998).
231. *Gross, A., C.-M. Wei, and M. Scheffler*: Poisoning of hydrogen dissociation at Pd(100) by adsorbed sulfur studied by ab-initio quantum dynamics and ab-initio molecular dynamics. *Surf. Sci.* **416**, L1095 (1998).

232. Kratzer, P., C.G. Morgan, and M. Scheffler: Density-functional theory studies on microscopic processes of GaAs growth. *Progr. Surf. Sci.* **59**, 135 (1998).
233. Kratzer, P., E. Pehlke, M. Scheffler, M.B. Raschke, and U. Höfer: Highly site-specific H₂ adsorption on vicinal Si(001) surfaces. *Phys. Rev. Lett.* **81**, 5596 (1998).
234. Moll, N., M. Scheffler, and E. Pehlke: Influence of surface stress on the equilibrium shape of strained quantum dots. *Phys. Rev. B* **58**, 4566 (1998).
235. Neugebauer, J., T. Zywietz, M. Scheffler, J.E. Northrup, and Ch.G. Van de Walle: Clean and As-covered zinc-blende GaN (001) surfaces: Novel surface structures and surfactant behavior. *Phys. Rev. Lett.* **80**, 3097 (1998).
236. Pohl, K., J.-H. Cho, K. Terakura, M. Scheffler, and E.W. Plummer: Anomalously large thermal expansion at the (0001) surface of beryllium without observable interlayer anharmonicity. *Phys. Rev. Lett.* **80**, 2853 (1998).
237. Ratsch, C., P. Ruggerone, and M. Scheffler: Study of strain and temperature dependence of metal epitaxy. In: *Morphological Organization in Epitaxial Growth and Removal*, Vol. 14. (Eds.) Z. Zhang, M.G. Lagally. World Scientific, Singapore 1998, 3.
238. Ratsch, C. and M. Scheffler: Density-functional theory calculations of hopping rates of surface diffusion. *Phys. Rev. B* **58**, 13163 (1998).
239. Ruggerone, P., A. Kley, and M. Scheffler: Bridging the length and time scales: from *ab initio* electronic structure calculations to macroscopic proportions. *Comments Cond. Mat. Phys.* **18**, 261 (1998).
240. Schwarz, G., A. Kley, J. Neugebauer, and M. Scheffler: Electronic and structural properties of vacancies on and below the GaP(110) surface. *Phys. Rev. B* **58**, 1392 (1998).
241. Schwegmann, S., A.P. Seitsonen, V. De Renzi, H. Dietrich, H. Bludau, M. Gierer, H. Over, K. Jacobi, M. Scheffler, and G. Ertl: Oxygen adsorption on the Ru(10̄10) surface: Anomalous coverage dependence. *Phys. Rev. B* **57**, 15487 (1998).
242. Stampfl, C., K. Kambe, R. Fasel, P. Aebi, and M. Scheffler: Theoretical analysis of the electronic structure of the stable and metastable *c*(2 × 2) phases of Na on Al(001): Comparison with angle-resolved ultraviolet photoemission spectra. *Phys. Rev. B* **57**, 15251 (1998).
243. Stampfl, C. and M. Scheffler: Coadsorption of CO and O on Ru(0001): A structural analysis by density functional theory. *Israel Journal of Chemistry* **38**, 409 (1998).
244. Wagner, F., Th. Laloyaux, and M. Scheffler: Errors in Hellmann-Feynman forces due to occupation-number broadening and how they can be corrected. *Phys. Rev. B* **57**, 2102 (1998).

245. Wang, X.-G., W. Weiss, Sh.K. Shaikhutdinov, M. Ritter, M. Petersen, F. Wagner, R. Schlögl, and M. Scheffler: The hematite (α -Fe₂O₃)(0001) surface: Evidence for domains of distinct chemistry. Phys. Rev. Lett. **81**, 1038 (1998).
246. Wei, C.M., A. Gross, and M. Scheffler: *Ab initio* calculation of the potential energy surface for the dissociation of H₂ on the sulfur-covered Pd(100) surface. Phys. Rev. B **57**, 15572 (1998).
247. Xie, J. and M. Scheffler: Structure and dynamics of Rh surfaces. Phys. Rev. B **57**, 4768 (1998).
248. Zywietz, T., J. Neugebauer, and M. Scheffler: Adatom diffusion at GaN(0001) and (0001̄) surfaces. Appl. Phys. Lett. **73**, 487 (1998).
249. Zywietz, T.K., J. Neugebauer, M. Scheffler, and J.E. Northrup: Novel reconstruction mechanisms: A comparison between group-III-nitrides and “traditional” III-V-semiconductors. HCM Newsletter (Ψ_k Network) **29** (1998).
250. Zywietz, T.K., J. Neugebauer, M. Scheffler, J.E. Northrup, and C.G. Van de Walle: Surface structures, surfactants and diffusion at cubic and wurtzite GaN. MRS Internet J. of Nitride Sem. Res. **3**, 26 (1998).
251. Bonn, M., S. Funk, Ch. Hess, D.N. Denzler, C. Stampfl, M. Scheffler, and M. Wolf, G. Ertl: Phonon- versus electron-mediated desorption and oxidation of CO on Ru(0001). SCIENCE **285**, 1042 (1999).
252. Chaka, A.M., and M. Scheffler: Quantum mechanics and the automobile: Tailoring the reactivity of sulfur for lubricant applications. ACS Preprints **44**, 297 (1999).
253. Eichler, A., J. Hafner, A. Gross, and M. Scheffler: Rotational effects in the dissociation of H₂ on metal surfaces studied by ab initio quantum-dynamics calculations. Chem. Phys. Lett. **311**, 1 (1999).
254. Eichler, A., J. Hafner, A. Gross, and M. Scheffler: Trends in the chemical reactivity of surfaces studied by ab initio quantum-dynamics calculations. Phys. Rev. B **59**, 13297 (1999).
255. Fuchs, M. and M. Scheffler: Ab initio pseudopotentials for electronic structure calculations of poly-atomic systems using density-functional theory. Comput. Phys. Commun. **119**, 67 (1999).
256. Ganduglia-Pirovano, M.V. and M. Scheffler: Structural and electronic properties of chemisorbed oxygen on Rh(111). Phys. Rev. B **59**, 15533 (1999).
257. Geelhaar, L., J. Márquez, K. Jacobi, A. Kley, P. Ruggerone, and M. Scheffler: A scanning tunneling microscopy study of the GaAs(112) surfaces. Microelectronics Journal **30**, 393 (1999).

258. Gonze, X. and M. Scheffler: Exchange and correlation kernels at the resonance frequency: Implications for excitation energies in density-functional theory. Phys. Rev. Lett. **82**, 4416 (1999).
259. Gross, A., M. Scheffler, M.J. Mehl, and D.A. Papaconstantopoulos: *Ab initio* based tight-binding Hamiltonian for the dissociation of molecules at surfaces. Phys. Rev. Lett. **82**, 1209 (1999).
260. Grosse, F., A. Kley, M. Scheffler, and R. Zimmermann: Self-organized growth on V-grooved substrates. In: Proc. 24th Int. Conf. on the Physics of Semiconductors. (Ed.) D. Gershoni. World Scientific, Singapore 1999, CD-ROM, Section VII: One and Zero Dimensional Systems; Subsection C: Mesoscopic Systems, No. 7.
261. Grosse, F., J. Neugebauer, and M. Scheffler: Phase stability and segregation of $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys. In: Proc. 24th Int. Conf. on the Physics of Semiconductors. (Ed.) D. Gershoni. World Scientific, Singapore 1999, CD-ROM, Section IX: Wide Band Gap Materials (Sic, GaN, II-VI, etc.); Subsection A: Growth, No. 3.
262. Harrison, N.M., X.-G. Wang, J. Muscat, and M. Scheffler: The influence of soft vibrational modes on our understanding of oxide surface structure. Faraday Discuss. **114**, 305 (1999).
263. Jacobi, K., J. Platen, C. Setzer, J. Márquez, L. Geelhaar, C. Meyne, W. Richter, A. Kley, P. Ruggerone, and M. Scheffler: Morphology, surface core-level shifts and surface energy of the faceted GaAs(112)A and $(\bar{1}\bar{1}\bar{2})\text{B}$ surfaces. Surf. Sci. **439**, 59 (1999).
264. Kim, H.W., J.R. Ahn, J.W. Chung, B.D. Yu, and M. Scheffler: Alkali metal (Li, K) induced reconstructions of the W(001) surface. Surf. Sci. **430**, L515 (1999).
265. Kratzer, P., C.G. Morgan, and M. Scheffler: Model for nucleation in GaAs homoepitaxy derived from first principles. Phys. Rev. B **59**, 15246 (1999).
266. LaBella, V.P., H. Yang, D.W. Bullock, P.M. Thibado, P. Kratzer, and M. Scheffler: Atomic structure of the GaAs(001)-(2×4) surface resolved using scanning tunneling microscopy and first-principles theory. Phys. Rev. Lett. **83**, 2989 (1999).
267. Liu, Q.K.K., N. Moll, M. Scheffler, and E. Pehlke: Equilibrium shapes and energies of coherent strained InP islands. Phys. Rev. B **60**, 17008 (1999).
268. Morgan, C.G., P. Kratzer, and M. Scheffler: Arsenic dimer dynamics during MBE growth: Theoretical evidence for a novel chemisorption state of As_2 molecules on GaAs surfaces. Phys. Rev. Lett. **82**, 4886 (1999).
269. Neugebauer, J., T.K. Zywietz, M. Scheffler, and J.E. Northrup: Surfaces and growth of group-III nitrides. In: Proc. 24th Int. Conf. on the Physics of Semiconductors. (Ed.) D. Gershoni. World Scientific, Singapore 1999, 235.
270. Nouvertné, F., U. May, M. Bamming, A. Rampe, U. Korte, G. Güntherodt, R. Pentcheva, and M. Scheffler: Atomic exchange processes and *bimodal* initial growth of Co/Cu(001). Phys. Rev. B **60**, 14382 (1999).

271. *Penev, E., P. Kratzer, and M. Scheffler*: Effect of the cluster size in modeling the H₂ desorption and dissociative adsorption on Si(001). *J. Chem. Phys.* **110**, 3986 (1999).
272. *Platen, J., A. Kley, C. Setzer, K. Jacobi, P. Ruggerone, and M. Scheffler*: The importance of high-index surfaces for the morphology of GaAs quantum dots. *J. Appl. Phys.* **85**, 3597 (1999).
273. *Stampfl, C., H.J. Kreuzer, S.H. Payne, H. Pfnür, and M. Scheffler*: First-principles theory of surface thermodynamics and kinetics. *Phys. Rev. Lett.* **83**, 2993 (1999).
274. *Stampfl, C., H.J. Kreuzer, S.H. Payne, and M. Scheffler*: Challenges in predictive calculations of processes at surfaces: surface thermodynamics and catalytic reactions. *Appl. Phys. A* **69**, 471 (1999).
275. *Stampfl, C. and M. Scheffler*: Density functional theory study of the catalytic oxidation of CO over transition metal surfaces. *Surf. Sci.* **433-435**, 119 (1999).
276. *Wang, L.G., P. Kratzer, M. Scheffler, and N. Moll*: Formation and stability of self-assembled coherent islands in highly mismatched heteroepitaxy. *Phys. Rev. Lett.* **82**, 4042 (1999).
277. *Xie, J., S. de Gironcoli, S. Baroni, and M. Scheffler*: First-principles calculation of the thermal properties of silver. *Phys. Rev. B* **59**, 965 (1999).
278. *Xie, J., S. de Gironcoli, S. Baroni, and M. Scheffler*: Temperature dependent surface relaxations of Ag(111). *Phys. Rev. B* **59**, 970 (1999).
279. *Zywietz, T.K., J. Neugebauer, and M. Scheffler*: The adsorption of oxygen at GaN surfaces. *Appl. Phys. Lett.* **74**, 1695 (1999).
280. *Ebert, Ph., K. Urban, L. Aballe, C.H. Chen, K. Horn, G. Schwarz, J. Neugebauer, and M. Scheffler*: Symmetric versus nonsymmetric structure of the phosphorus vacancy on InP(110). *Phys. Rev. Lett.* **84**, 5816 (2000).
281. *Fichthorn, K.A. and M. Scheffler*: Island nucleation in thin-film epitaxy: A first-principles investigation. *Phys. Rev. Lett.* **84**, 5371 (2000).
282. *Gross, A. and M. Scheffler*: Dynamics of hydrogen dissociation at the sulfur-covered Pd(100) surface. *Phys. Rev. B* **61**, 8425 (2000).
283. *Horn, K. and M. Scheffler (Eds.)*: *Handbook of Surface Science*, Vol. 2 (Electronic Structure). Elsevier Science, Amsterdam 2000.
284. *LaBella, V.P., D.W. Bullock, Z. Ding, C. Emery, P.M. Thibado, P. Kratzer, M. Scheffler*: A novel imaging mechanism to determine the atomic structure of the GaAs(001)-(2×4) surface. *Omicron Newsletter* **4**, No. 2, 4 (2000).
285. *Lee, S.-H., W. Moritz, and M. Scheffler*: GaAs(001) surface under conditions of low As pressure: Evidence for a novel surface geometry. *Phys. Rev. Lett.* **85**, 3890 (2000).

286. *Neugebauer, J., T. Zywietz, M. Scheffler, and J. Northrup*: Theory of surfaces and interfaces of group III-nitrides. *Appl. Surf. Sci.* **159-160**, 355 (2000).
287. *Pentcheva, R. and M. Scheffler*: Stable and metastable structures of Co on Cu(001): An *ab initio* study. *Phys. Rev. B* **61**, 2211 (2000).
288. *Petersen, M., F. Wagner, L. Hufnagel, M. Scheffler, P. Blaha, and K. Schwarz*: Improving the efficiency of FP-LAPW calculations. *Comp. Phys. Commun.* **126**, 294 (2000).
289. *Scheffler, M., P. Kratzer, and L.G. Wang*: *Ab initio* thermodynamics and statistics of semiconductor growth, and self-assembly of quantum dots. In: Proc. 4th Symposium on Atom-Scale Surface and Interface Dynamics, No. 9: JSPS Research for the Future Program “Atom-Scale Surface and Interface Dynamics”. Japan Society for the Promotion of Science, March 2000, 3.
290. *Scheffler, M. and C. Stampfl*: Theory of adsorption on metal substrates. In: *Handbook of Surface Science*, Vol. 2: Electronic Structure. (Eds.) K. Horn, M. Scheffler. Elsevier Science, Amsterdam 2000, 286.
291. *Wang, L.G., P. Kratzer, and M. Scheffler*: Energetics of InAs thin films and islands on the GaAs(001) substrate. *Jpn. J. Appl. Phys.* **39**, 4298 (2000).
292. *Wang, L.G., P. Kratzer, N. Moll, and M. Scheffler*: Size, shape, and stability of InAs quantum dots on the GaAs(001) substrate. *Phys. Rev. B* **62**, 1897 (2000).
293. *Wang, X.-G., A. Chaka, and M. Scheffler*: Effect of the environment on $\alpha\text{-Al}_2\text{O}_3$ (0001) surface structures. *Phys. Rev. Lett.* **84**, 3650 (2000).
294. *Dohmen, R., J. Pichlmeier, M. Petersen, F. Wagner, and M. Scheffler*: Parallel FP-LAPW for distributed-memory machines. *Computing in Science & Engineering* **3**, No. 4, 18 (2001).
295. *Ebert, Ph., P. Quadbeck, K. Urban, B. Henninger, K. Horn, G. Schwarz, J. Neugebauer, and M. Scheffler*: Identification of surface anion antisite defects in (110) surfaces of III-V semiconductors. *Appl. Phys. Lett.* **79**, 2877 (2001).
296. *Feibelman, P.J., B. Hammer, J.K. Nørskov, F. Wagner, M. Scheffler, R. Stumpf, R. Watwe, and J. Dumesic*: The CO/Pt(111) puzzle. *J. Phys. Chem. B* **105**, 4018 (2001).
297. *Fichthorn, K.A. and M. Scheffler*: Substrate-mediated interaction on Ag(111) surfaces from first principles. In: *Collective Diffusion on Surfaces: Collective Behaviour and the Role of Adatom Interactions*. (Eds.) M.C. Tringides and Z. Chvoj. Kluwer, Dordrecht 2001, 225.
298. *Ganduglia-Pirovano, M.V., M. Scheffler, A. Baraldi, S. Lizzit, G. Comelli, G. Paolucci, and R. Rosei*: Oxygen induced Rh $3d_{5/2}$ surface core-level shifts on Rh(111). *Phys. Rev. B* **63**, 205415 (2001).

299. *Healy, S.B., C. Filippi, P. Kratzer, E. Penev, and M. Scheffler*: The role of electronic correlation in the Si(100) reconstruction: a quantum Monte Carlo study. Phys. Rev. Lett. **87**, 016105 (2001).
300. *Kratzer, P. and M. Scheffler*: Surface Knowledge: Toward a Predictive Theory of Materials. Computing in Science & Engineering **3**, No. 6 (Nov./Dec.), 16 (2001).
301. *Lizzit, S., A. Baraldi, A. Groso, K. Reuter, M.V. Ganduglia-Pirovano, C. Stampfl, M. Scheffler, M. Stichler, C. Keller, W. Wurth, and D. Menzel*: Surface core level shifts of clean and oxygen covered Ru(0001). Phys. Rev. B **63**, 205419 (2001).
302. *Márquez, J., P. Kratzer, L. Geelhaar, K. Jacobi, and M. Scheffler*: Atomic structure of the stoichiometric GaAs(114) surface. Phys. Rev. Lett. **86**, 115 (2001).
303. *Penev, E., P. Kratzer, and M. Scheffler*: Effect of strain on surface diffusion in semiconductor heteroepitaxy. Phys. Rev. B **64**, 085401 (2001).
304. *Reuter K. and M. Scheffler*: Composition, structure, and stability of RuO₂(110) as a function of oxygen pressure. Phys. Rev. B **65**, 035406 (2001); Phys. Rev. B **75**, 049901(E) (2007).
305. *Reuter, K. and M. Scheffler*: Surface core-level shifts at an oxygen-rich Ru surface: O/Ru(0001) vs. RuO₂(110). Surf. Sci. **490**, 20 (2001).
306. *Schwarz, G., J. Neugebauer, and M. Scheffler*: Point defects on III-V semiconductor surfaces. In: Proc. 25th Int. Conf. Phys. Semicond. (Eds.) N. Miura, T. Ando. Springer Proc. in Physics, Vol. 87, Springer, Berlin/Heidelberg 2001, 1377.
307. *Tatarczyk, K., A. Schindlmayr, and M. Scheffler*: Exchange-correlation kernels for excited states in solids. Phys. Rev. B **63**, 235106 (2001).
308. *Wang, L.G., P. Kratzer, and M. Scheffler, Q.K.K. Liu*: Island dissolution during capping layer growth interruption. Appl. Phys. A **73**, 161 (2001).
309. *Erwin, S.C., S.-H. Lee, and M. Scheffler*: First-principles study of nucleation, growth, and interface structure on Fe/GaAs. Phys. Rev. B **65**, 205422 (2002).
310. *Fichthorn, K.A., M.L. Merrick, R. Pentcheva, and M. Scheffler*: Island nucleation in metal thin-film growth. In: Atomistic Aspects of Epitaxial Growth. (Eds.) M. Kotrla, N.I. Papanicolaou, D.D. Vvedensky, and L.T. Wille. Kluwer, Dordrecht 2002, 87.
311. *Fichthorn, K.A., M.L. Merrick, and M. Scheffler*: A kinetic Monte Carlo investigation of island nucleation and growth in thin-film epitaxy in the presence of substrate-mediated interactions. Appl. Phys. A **75**, 17 (2002).
312. *Filippi, C., S.B. Healy, P. Kratzer, E. Pehlke, and M. Scheffler*: Quantum Monte Carlo calculations of H₂ dissociation on Si(001). Phys. Rev. Lett. **89**, 166102 (2002).

313. *Fuchs, M., J.L.F. Da Silva, C. Stampfl, J. Neugebauer, and M. Scheffler*: Cohesive properties of group-III nitrides: A comparative study of all-electron and pseudopotential calculations using the generalized gradient approximation. *Phys. Rev. B* **65**, 245212 (2002).
314. *Ganduglia-Pirovano, M.V., K. Reuter, and M. Scheffler*: Stability of subsurface oxygen at Rh(111). *Phys. Rev. B* **65**, 245426 (2002).
315. *Hedström, M., A. Schindlmayr, and M. Scheffler*: Quasiparticle calculations for point defects on semiconductor surfaces. *phys. stat. sol. (b)* **234**, 346 (2002).
316. *Kratzer, P., E. Penev, and M. Scheffler*: First-principles studies of kinetics in epitaxial growth of III-V semiconductors. *Appl. Phys. A* **75**, 79 (2002).
317. *Kratzer, P. and M. Scheffler*: Reaction-limited island nucleation in molecular beam epitaxy of compound semiconductors. *Phys. Rev. Lett.* **88**, 036102 (2002).
318. *Kroes, G.-J., A. Gross, E.-J. Baerends, M. Scheffler, and D.A. McCormack*: Quantum theory of dissociative chemisorption on metal surfaces. *Acc. Chem. Res.* **35**, 193 (2002).
319. *Lee, S.M., S.-H. Lee, and M. Scheffler*: Comment on “Anomalous mobility of strongly bound surface species: Cl on GaAs(001)-c(8 x 2)”. *Phys. Rev. Lett.* **89**, 239601 (2002).
320. *Li, W.X., C. Stampfl, and M. Scheffler*: Oxygen adsorption on Ag(111): A density-functional theory investigation. *Phys. Rev. B* **65**, 075407 (2002).
321. *Pentcheva, R. and M. Scheffler*: Initial adsorption of Co on Cu(001): A first-principles investigation. *Phys. Rev. B* **65**, 155418 (2002).
322. *Reuter K., M.V. Ganduglia-Pirovano, C. Stampfl, and M. Scheffler*: Metastable precursors during the oxidation of the Ru(0001) surface. *Phys. Rev. B* **65**, 165403 (2002).
323. *Reuter, K., C. Stampfl, M.V. Ganduglia-Pirovano, and M. Scheffler*: Atomistic description of oxide formation on metal surfaces: the example of ruthenium. *Chem. Phys. Lett.* **352**, 311 (2002).
324. *Scheffler, M. and P. Kratzer*: Ab initio thermodynamics and statistical mechanics of diffusion, growth, and self-assembly of quantum dots. In: *Atomistic Aspects of Epitaxial Growth*. (Eds.) M. Kotrla, N.I. Papanicolaou, D.D. Vvedensky, and L.T. Wille. Kluwer Academic Publishers, The Netherlands 2002, 355.
325. *Stampfl, C., M.V. Ganduglia-Pirovano, K. Reuter, and M. Scheffler*: Catalysis and corrosion: the theoretical surface-science context. *Surf. Sci.* **500**, 368 (2002).
326. *Stampfl, C. and M. Scheffler*: Energy barriers and chemical properties in the coadsorption of carbon monoxide and oxygen on Ru(0001). *Phys. Rev. B* **65**, 155417 (2002).

327. *Todorova, M., W.X. Li, M.V. Ganduglia-Pirovano, C. Stampfl, K. Reuter, and M. Scheffler*: Role of sub-surface oxygen in oxide formation at transition metal surfaces. *Phys. Rev. Lett.* **89**, 096103 (2002).
328. *Wang, X.-G., J.R. Smith, and M. Scheffler*: Effect of hydrogen on $\text{Al}_2\text{O}_3/\text{Cu}$ interfacial structure and adhesion. *Phys. Rev. B* **66**, 073411 (2002).
329. *Da Silva, J. L.F., C. Stampfl, and M. Scheffler*: Adsorption of Xe atoms on metal surfaces: New insights from first-principles calculations. *Phys. Rev. Lett.* **90**, 066104 (2003).
330. *Fichthorn, K.A., M.L. Merrick, and M. Scheffler*: Nanostructures at surfaces from substrate-mediated interactions. *Phys. Rev. B* **68**, 041404(R) (2003).
331. *Ireta, J., J. Neugebauer, M. Scheffler, A. Rojo, and M. Galván*: Density functional theory study of the cooperativity of hydrogen bonds in finite and infinite α -helices. *J. Phys. Chem. B* **107**, 1432 (2003); *J. Phys. Chem. B* **107**, 9616(E) (2003).
332. *Kratzer, P., E. Penev, and M. Scheffler*: Understanding the growth mechanisms of GaAs and InGaAs thin films by employing first-principles calculations. *Appl. Surf. Sci.* **216**, 436 (2003).
333. *Li, W.X., C. Stampfl, and M. Scheffler*: Insights into the function of silver as an oxidation catalyst by ab initio atomistic thermodynamics. *Phys. Rev. B* **68**, 165412 (2003).
334. *Li, W.X., C. Stampfl, and M. Scheffler*: Subsurface oxygen and surface oxide formation at Ag(111): A density-functional theory investigation. *Phys. Rev. B* **67**, 045408 (2003).
335. *Li, W.X., C. Stampfl, and M. Scheffler*: Why is a noble metal catalytically active? The role of the O-Ag interaction in the function of silver as an oxidation catalyst. *Phys. Rev. Lett.* **90**, 256102 (2003).
336. *Neugebauer, J., T.K. Zywietz, M. Scheffler, J.E. Northrup, H. Chen, and R.M. Feenstra*: Adatom kinetics on and below the surface: The existence of a new diffusion channel. *Phys. Rev. Lett.* **90**, 056101 (2003).
337. *Pentcheva, R., K.A. Fichthorn, M. Scheffler, T. Bernhard, R. Pfandzelter, and H. Winter*: Non-Arrhenius behavior of the island density in metal heteroepitaxy: Co on Cu(001). *Phys. Rev. Lett.* **90**, 076101 (2003).
338. *Reuter K. and M. Scheffler*: Composition and structure of the $\text{RuO}_2(110)$ surface in an O_2 and CO environment: Implications for the catalytic formation of CO_2 . *Phys. Rev. B* **68**, 045407 (2003).
339. *Reuter K. and M. Scheffler*: First-principles atomistic thermodynamics for oxidation catalysis: Surface phase diagrams and catalytically interesting regions. *Phys. Rev. Lett.* **90**, 046103 (2003).

340. *Santoprete, R., B. Koiller, R.B. Capaz, P. Kratzer, Q.K.K. Liu, and M. Scheffler*: Tight-binding study of the influence of the strain on the electronic properties of InAs/GaAs quantum dots. *Phys. Rev. B* **68**, 235311 (2003).
341. *Scharoch, P., J. Neugebauer and M. Scheffler*: Al(111)-($\sqrt{3} \times \sqrt{3}$)R30: On-top versus substitutional adsorption for Rb and K. *Phys. Rev. B* **68**, 035403 (2003).
342. *Scheffler, M. and P. Weinberger (Eds.)*: Walter Kohn - Personal stories and anecdotes told by friends and collaborators. Springer-Verlag, Berlin Heidelberg New York 2003. ISBN 3-540-00805-5.
343. *Sun, Q., K. Reuter, and M. Scheffler*: Effect of a humid environment on the surface structure of RuO₂(110). *Phys. Rev. B* **67**, 205424 (2003).
344. *Todorova, M., E. Lundgren, V. Blum, A. Mikkelsen, S. Gray, J. Gustafson, M. Borg, J. Rogal, K. Reuter, J.N. Andersen, and M. Scheffler*: The Pd(100)-($\sqrt{5} \times \sqrt{5}$)R27°-O surface oxide revisited. *Surf. Sci.* **541**, 101 (2003).
345. *Wang, J., C.Y. Fan, Q. Sun, K. Reuter, K. Jacobi, M. Scheffler, and G. Ertl*: Surface coordination chemistry: Dihydrogen versus hydride complexes on RuO₂(110). *Angew. Chem.* **115**, 2201 (2003); *Angew. Chem. Int. Ed.* **42**, 2151 (2003).
346. *Wang, X.-G., J.R. Smith, and M. Scheffler*: Adhesion of copper and alumina from first principles. *J. Am. Ceram. Soc.* **86**, 696 (2003).
347. *Duplock, E., M. Scheffler, and P.J.D. Lindan*: Hallmark of perfect graphene. *Phys. Rev. Lett.* **92**, 225502 (2004).
348. *Fichthorn, K. and M. Scheffler*: Nanophysics – A step up to self-assembly. *Nature* **429**, 617 (2004).
349. *Fielicke, A., A. Kirilyuk, C. Ratsch, J. Behler, M. Scheffler, G. von Helden, and G. Meijer*: Structure determination of isolated metal clusters via far-infrared spectroscopy. *Phys. Rev. Lett.* **93**, 023401 (2004).
350. *Ireta, J., J. Neugebauer, and M. Scheffler*: On the accuracy of DFT for describing hydrogen bonds: Dependence on the bond directionality. *J. Chem. Phys. A* **108**, 5692 (2004).
351. *Lee, S.M., S.-H. Lee, and M. Scheffler*: Adsorption and diffusion of a Cl adatom on the GaAs(001)-c(8×2)ζ surface. *Phys. Rev. B* **69**, 125317 (2004).
352. *Lorenz, S., A. Gross, and M. Scheffler*: Representing high-dimensional potential-energy surfaces for reactions at surfaces by neural networks. *Chem. Phys. Lett.* **395**, 210 (2004).
353. *Lundgren, E., J. Gustafson, A. Mikkelsen, J.N. Andersen, A. Stierle, H. Dosch, M. Todorova, J. Rogal, K. Reuter, and M. Scheffler*: Kinetic hindrance during the initial oxidation of Pd(100) at ambient pressures. *Phys. Rev. Lett.* **92**, 046101 (2004).

354. *Penev, E., P. Kratzer, and M. Scheffler*: Atomic structure of the GaAs(001)-c(4 × 4) surface: First-principles evidence for diversity of heterodimer motifs. *Phys. Rev. Lett.* **93**, 146102 (2004).
355. *Penev, E., S. Stojković, P. Kratzer, and M. Scheffler*: Anisotropic diffusion of In adatoms on pseudomorphic In_xGa_{1-x}As(001) films: First-principles total energy calculations. *Phys. Rev. B* **69**, 115335 (2004).
356. *Reuter K., D. Frenkel, and M. Scheffler*: The steady state of heterogeneous catalysis, studied by first-principles statistical mechanics. *Phys. Rev. Lett.* **93**, 116105 (2004).
357. *Reuter K. and M. Scheffler*: Oxide formation at the surface of late 4d transition metals: insights from first-principles atomistic thermodynamics. *Appl. Phys. A* **78**, 793 (2004).
358. *Rogal, J., K. Reuter, and M. Scheffler*: Thermodynamic stability of PdO surfaces. *Phys. Rev. B* **69**, 075421 (2004).
359. *Sun, Q., K. Reuter, and M. Scheffler*: Hydrogen adsorption at RuO₂(110): Density-functional calculations. *Phys. Rev. B* **70**, 235402 (2004).
360. *Todorova, M., K. Reuter, and M. Scheffler*: Oxygen overlayers on Pd(111) studied by density functional theory. *J. Phys. Chem. B* **108**, 14477 (2004).
361. *Wu, H., M. Hortamani, P. Kratzer, and M. Scheffler*: First-principles study of ferromagnetism in epitaxial Si-Mn thin films on Si(001). *Phys. Rev. Lett.* **92**, 237202 (2004).
362. *Yu, D.K. and M. Scheffler*: First-principles study of low-index surfaces of lead. *Phys. Rev. B* **70**, 155417 (2004).
363. *Behler, J., B. Delley, S. Lorenz, K. Reuter, and M. Scheffler*: Dissociation of O₂ at Al(111): The role of spin selection rules. *Phys. Rev. Lett.* **94**, 036104 (2005).
364. *Borg, M., C. Stampfl, A. Mikkelsen, J. Gustafson, E. Lundgren, M. Scheffler, and J.N. Andersen*: Density of configurational states from first-principles: The phase diagram of Al-Na surface alloys. *ChemPhysChem* **6**, 1923 (2005).
365. *Carlsson, J. and M. Scheffler*: Curvature effects on vacancies in nanotubes. In: Electronic Properties of Novel Nanostructures: Proc. of the XIX International Winterschool/Euroconference on Electronic Properties of Novel Materials, Kirchberg, Austria (IWEPNM 2005). (Eds.) H. Kuzmany, J. Fink, M. Mehring, S. Roth. AIP Conference Proceedings **786**. American Institute of Physics, New York 2005, 432. ISBN 0-7354-0275-2.
366. *Da Silva, J.L.F., C. Stampfl, and M. Scheffler*: Xe adsorption on metal surfaces: First-principles investigations. *Phys. Rev. B* **72**, 075424 (2005).

367. *Fonin, M., R. Pentcheva, Yu.S. Dedkov, M. Sperlich, D.V. Vyalikh, M. Scheffler, U. Rüdiger, and G. Güntherodt*: Surface electronic structure of the $\text{Fe}_3\text{O}_4(100)$: Evidence of a half-metal to metal transition. *Phys. Rev. B* **72**, 104436 (2005).
368. *Hashemifar, S.J., P. Kratzer, and M. Scheffler*: Preserving half-metalllicity at the Heusler alloy $\text{Co}_2\text{MnSi}(001)$ surface: A density functional theory study. *Phys. Rev. Lett.* **94**, 096402 (2005).
369. *Ireta, J., J. Neugebauer, M. Scheffler, A. Rojo, and M. Galván*: Structural transitions in the polyalanine α -helix under uniaxial strain. *J. Am. Chem. Soc.* **127**, 17241 (2005).
370. *Michaelides, A., K. Reuter, and M. Scheffler*: When seeing is not believing: Oxygen on $\text{Ag}(111)$, a simple adsorption system? *J. Vac. Sci. Technol. A* **23**, 1487 (2005).
371. *Pentcheva, R., F. Wagner, W. Moritz, and M. Scheffler*: Structure, energetics and properties of $\text{Fe}_3\text{O}_4(001)$ from first principles. In: *High Performance Computing in Science and Engineering*, Munich 2004. (Eds.) S. Wagner, W. Hanke, A. Bode, F. Durst. Springer-Verlag Berlin-Heidelberg, 2005, 375. ISBN 3-540-44326-6.
372. *Pentcheva, R., F. Wendler, H.L. Meyerheim, W. Moritz, N. Jedrecy, and M. Scheffler*: Jahn-Teller stabilization of a “polar” metal oxide surface: $\text{Fe}_3\text{O}_4(001)$. *Phys. Rev. Lett.* **94**, 126101 (2005).
373. *Qteish, A., A.I. Al-Sharif, M. Fuchs, M. Scheffler, S. Boeck, and J. Neugebauer*: Exact-exchange calculations of the electronic structure of AlN, GaN and InN. *Comp. Phys. Comm.* **169**, 28 (2005).
374. *Qteish, A., A.I. Al-Sharif, M. Fuchs, M. Scheffler, S. Boeck, and J. Neugebauer*: Role of semicore states in the electronic structure of group-III nitrides: An exact-exchange study. *Phys. Rev. B* **72**, 155317 (2005).
375. *Ratsch, C., A. Fielicke, J. Behler, M. Scheffler, G. von Helden, and G. Meijer*: Structure determination of small metal clusters by density-functional theory and comparison with experimental far-infrared spectra. In: *Technical Proceedings of the 2005 NSTI Nanotechnology Conference and Trade Show. Nanotech 2005* **2**, 1 (2005).
376. *Ratsch C., A. Fielicke, A. Kirilyuk, J. Behler, G. von Helden, G. Meijer, and M. Scheffler*: Structure determination of small vanadium clusters by density-functional theory in comparison with experimental far-infrared spectra. *J. Chem. Phys.* **122**, 124302 (2005).
377. *Reuter K., C. Stampfl, and M. Scheffler*: *Ab initio* atomistic thermodynamics and statistical mechanics of surface properties and functions. In: *Handbook of Materials Modeling*, Vol. 1. (Ed.) Sidney Yip. Springer Berlin Heidelberg 2005, 149. ISBN 1-4020-3287-0.

378. Rinke, P., A. Qteish, J. Neugebauer, C. Freysoldt, and M. Scheffler: Combining GW calculations with exact-exchange density-functional theory: an analysis of valence-band photoemission for compound semiconductors. *New J. Phys.* **7**, 126 (2005).
379. Santoprete, R., B. Koiller, R.B. Capaz, P. Kratzer, and M. Scheffler: Strain effects on the electronic and optical properties of InAs/GaAs quantum dots: Tight-binding study. In: *Physics of Semiconductors: 27th Int. Conf. on the Physics of Semiconductors (ICPS-27)*. (Eds.) J. Menéndez, C.G. Van de Walle. AIP Conf. Proc. **772**. American Institute of Physics 2005, 745-746. ISBN 0-7354-0257-4.
380. Todorova, M., K. Reuter, and M. Scheffler: Density-functional theory study of the initial oxygen incorporation in Pd(111). *Phys. Rev. B* **71**, 195403 (2005).
381. Wu, H., P. Kratzer, and M. Scheffler: *Ab initio* study of transition-metal silicide films on Si(001). In: *Physics of Semiconductors: 27th Int. Conf. on the Physics of Semiconductors (ICPS-27)*. (Eds.) J. Menéndez, C.G. Van de Walle. AIP Conf. Proc. **772**. American Institute of Physics 2005, 311. ISBN 0-7354-0257-4.
382. Wu, H., P. Kratzer, and M. Scheffler: First-principles study of thin magnetic transition-metal silicide films on Si(001). *Phys. Rev. B* **72**, 144425 (2005).
383. Carlsson, J.M. and M. Scheffler: Structural, electronic, and chemical properties of nanoporous carbon. *Phys. Rev. Lett.* **96**, 046806 (2006).
384. Chakrabarti, A., P. Kratzer, and M. Scheffler: Surface reconstructions and atomic ordering in $\text{In}_x\text{Ga}_{1-x}\text{As}(001)$ films: A density-functional theory study. *Phys. Rev. B* **74**, 245328 (2006).
385. Da Silva, J.L.F., C. Stampfl, and M. Scheffler: Converged properties of clean metal surfaces by all-electron first-principles calculations. *Surf. Sci.* **600**, 703 (2006).
386. Hedström, M., A. Schindlmayr, G. Schwarz, and M. Scheffler: Quasiparticle corrections to the electronic properties of anion vacancies at GaAs(110) and InP(110). *Phys. Rev. Lett.* **97**, 226401 (2006).
387. Hortamani, M., H. Wu, P. Kratzer, and M. Scheffler: Epitaxy of Mn on Si(001): Adsorption, surface diffusion, and magnetic properties studied by density-functional theory. *Phys. Rev. B* **74**, 205305 (2006).
388. Kiejna, A., G. Kresse, J. Rogal, A. De Sarkar, K. Reuter, and M. Scheffler: Comparison of the full-potential and frozen-core approximation approaches to density-functional calculations of surfaces. *Phys. Rev. B* **73**, 035404 (2006).
389. Li, B., A. Michaelides, and M. Scheffler: “Textbook” adsorption at “nontextbook” adsorption sites: Halogen atoms on alkali halide surfaces. *Phys. Rev. Lett.* **97**, 046802 (2006).

390. *Lorenz, S., M. Scheffler, and A. Gross*: Descriptions of surface chemical reactions using a neural network representation of the potential-energy surface. *Phys. Rev. B* **73**, 115431 (2006).
391. *Nørskov, J.K., M. Scheffler, and H. Toulhoat*: Density-functional theory in surface science and heterogeneous catalysis. *MRS Bulletin* **31**, 669 (2006).
392. *Qteish, A., P. Rinke, M. Scheffler, and J. Neugebauer*: Exact-exchange-based quasiparticle energy calculations for the band gap, effective masses, and deformation potentials of ScN. *Phys. Rev. B* **74**, 245208 (2006).
393. *Reuter, K. and M. Scheffler*: First-principles kinetic Monte Carlo simulations for heterogeneous catalysis: Application to the CO oxidation at RuO₂(110). *Phys. Rev. B* **73**, 045433 (2006).
394. *Rinke, P., M. Scheffler, A. Qteish, M. Winkelnkemper, D. Bimberg, and J. Neugebauer*: Band gap and band parameters of InN and GaN from quasiparticle energy calculations based on exact-exchange density-functional theory. *Appl. Phys. Lett.* **89**, 161919 (2006).
395. *Schnadt, J., A. Michaelides, J. Knudsen, R.T. Vang, K. Reuter, E. Lægsgaard, M. Scheffler, and F. Besenbacher*: Revisiting the structure of the $p(4 \times 4)$ surface oxide on Ag(111). *Phys. Rev. Lett.* **96**, 146101 (2006).
396. *Yu, D.K., H.P. Bonzel, and M. Scheffler*: Orientation-dependent surface and step energies of Pb from first principles. *Phys. Rev. B* **74**, 115408 (2006).
397. *Yu, D.K., H.P. Bonzel, and M. Scheffler*: The stability of vicinal surfaces and the equilibrium crystal shape of Pb by first principles theory. *New Journal of Physics* **8** (65), 1 (2006).
398. *Yu, D.K., M. Scheffler, and M. Persson*: Quantum size effect in Pb(100) films: Role of symmetry and implications for film growth. *Phys. Rev. B* **74**, 113401 (2006).
399. *Behler, J., B. Delley, K. Reuter, and M. Scheffler*: Nonadiabatic potential-energy surfaces by constrained density-functional theory. *Phys. Rev. B* **75**, 115409 (2007).
400. *Bonzel, H.P., D.K. Yu, and M. Scheffler*: The three-dimensional equilibrium crystal shape of Pb: Recent results of theory and experiment. *Appl. Phys. A* **87**, 391 (2007).
401. *Buecking, N., M. Scheffler, P. Kratzer, and A. Knorr*: Theory of optical excitation and relaxation phenomena at semiconductor surfaces: linking density functional and density matrix theory. *Appl. Phys. A* **88**, 505 (2007).
402. *Freysoldt, C., P. Eggert, P. Rinke, A. Schindlmayr, R.W. Godby, M. Scheffler*: Dielectric anisotropy in the GW space-time method. *Comp. Phys. Comm.* **176**, 1 (2007).

403. *Freysoldt, C., P. Rinke, and M. Scheffler*: Ultrathin oxides: Bulk-oxide-like model surfaces or unique films? *Phys. Rev. Lett.* **99**, 086101 (2007).
404. *Friák, M., A. Schindlmayr, and M. Scheffler*: *Ab initio* study of half-metal to metal transition in strained magnetite. *New J. Phys.* **9** (5), 1 (2007).
405. *Hammerschmidt, T., P. Kratzer, and M. Scheffler*: Elastic response of cubic crystals to biaxial strain: Analytic results and comparison to density functional theory for InAs. *Phys. Rev. B* **75**, 235328 (2007).
406. *Hortamani, M., P. Kratzer, and M. Scheffler*: Density-functional study of Mn monosilicide on the Si(111) surface: Film formation versus island nucleation. *Phys. Rev. B* **76**, 235426 (2007).
407. *Hu, Q.-M., K. Reuter, and M. Scheffler*: Towards an exact treatment of exchange and correlation in materials: Application to the “CO adsorption puzzle” and other systems. *Phys. Rev. Lett.* **98**, 176103 (2007); *Phys. Rev. Lett.* **99**, 169903(E) (2007).
408. *Knözinger, H. und M. Scheffler*: Expedition zwischen Physik und Chemie: Chemie-Nobelpreis 2007 an Gerhard Ertl. *Physik Journal* **6**, Nr. 12, 27 (2007).
409. *Kratzer, P., S.J. Hashemifar, H. Wu, M. Hortamani, and M. Scheffler*: Transition-metal silicides as materials for magnet-semiconductor heterostructures. *J. Appl. Phys.* **101**, 081725 (2007).
410. *Krause, M.R., A.J. Stollenwerk, J. Reed, V.P. LaBella, M. Hortamani, P. Kratzer, and M. Scheffler*: Electronic structure changes of Si(001)-(2×1) from subsurface Mn observed by STM. *Phys. Rev. B* **75**, 205326 (2007).
411. *Li, B., A. Michaelides, and M. Scheffler*: Density functional theory study of flat and stepped NaCl(001). *Phys. Rev. B* **76**, 075401 (2007).
412. *Rinke, P., A. Qteish, J. Neugebauer, and M. Scheffler*: Exciting prospects for solids: Exact-exchange based functionals meet quasiparticle energy calculations. Ψ_k Newsletter No. 79, 163 (2007).
413. *Rogal, J., K. Reuter, and M. Scheffler*: CO oxidation at Pd(100): A first-principles constrained thermodynamics study. *Phys. Rev. B* **75**, 205433 (2007).
414. *Rogal, J., K. Reuter, and M. Scheffler*: First-principles statistical mechanics study of the stability of a subnanometer thin surface oxide in reactive environments: CO oxidation at Pd(100). *Phys. Rev. Lett.* **98**, 046101 (2007).
415. *Santoprete, R., P. Kratzer, M. Scheffler, R.B. Capaz, and B. Koiller*: Effect of post-growth annealing on the optical properties of InAs/GaAs quantum dots: A tight-binding study. *J. Appl. Phys.* **102**, 023711 (2007).
416. *Santra, B., A. Michaelides, and M. Scheffler*: On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters: Benchmarks approaching the complete basis set limit. *J. Chem. Phys.* **127**, 184104 (2007).

417. Scheffler, M. and W.-D. Schneider (Eds.): Focus on Advances in Surface and Interface Science. New J. Phys. **9**, No. 10, IOP Publishing Ltd and Deutsche Physikalische Gesellschaft (October 2007). doi:10.1088/1367-2630/9/10/E07.
418. Schindlmayr, A. and M. Scheffler: Quasiparticle calculations for point defects at semiconductor surfaces. In: Theory of Defects in Semiconductors. (Eds.) D.A. Drabold, S.K. Estreicher. Springer Series **104** “Topics in Applied Physics”, Springer Berlin Heidelberg 2007, 165. ISBN 978-3-540-33400-2.
419. Temel, B., H. Meskine, K. Reuter, M. Scheffler, and H. Metiu: Does phenomenological kinetics provide an adequate description of heterogeneous catalytic reactions? J. Chem. Phys. **126**, 204711 (2007).
420. Wu, H., P. Kratzer, and M. Scheffler: Density-functional theory study of half-metallic heterostructures: Interstitial Mn in Si. Phys. Rev. Lett. **98**, 117202 (2007).
421. Behler, J., K. Reuter, and M. Scheffler: Nonadiabatic effects in the dissociation of oxygen molecules at the Al(111) surface. Phys. Rev. B **77**, 115421 (2008).
422. Buecking, N., S. Butscher, M. Richter, C. Weber, S. Declair, M. Woerner, K. Reimann, P. Kratzer, M. Scheffler, and A. Knorr: Theory of electron-phonon interactions on nanoscales: semiconductor surfaces and two dimensional electron gases. Proc. of SPIE **6892**, 689209 (2008).
423. Buecking, N., M. Scheffler, P. Kratzer, and A. Knorr: Linking density functional and density-matrix theory: Picosecond electron relaxation at the Si(100) surface. Phys. Rev. B **77**, 233305 (2008).
424. Freysoldt, C., P. Eggert, P. Rinke, A. Schindlmayr, and M. Scheffler: Screening in two dimensions: *GW* calculations for surfaces and thin films using the repeated-slab approach. Phys. Rev. B **77**, 235428 (2008).
425. Gómez-Abal, R., X. Li, M. Scheffler, and C. Ambrosch-Draxl: Influence of the core-valence interaction and of the pseudopotential approximation on the electron self-energy in semiconductors. Phys. Rev. Lett. **101**, 106404 (2008).
426. Hammerschmidt, T., P. Kratzer, and M. Scheffler: Analytic many-body potential for InAs/GaAs surfaces and nanostructures: Formation energy of InAs quantum dots. Phys. Rev. B **77**, 235303 (2008); Phys. Rev. B **81**, 159905(E) (2010).
427. Hortamani, M., L. Sandratskii, P. Kratzer, I. Mertig, and M. Scheffler: Exchange interactions and critical temperature of bulk and thin films of MnSi: A density functional theory study. Phys. Rev. B **78**, 104402 (2008).
428. Kitchin, J.R., K. Reuter, and M. Scheffler: Alloy surface segregation in reactive environments: First-principles atomistic thermodynamics study of Ag₃Pd(111) in oxygen atmospheres. Phys. Rev. B **77**, 075437 (2008).
429. Li, B., A. Michaelides, and M. Scheffler: How strong is the bond between water and salt? Surf. Sci. **602**, L135 (2008).

430. *Pentcheva, R., W. Moritz, J. Rundgren, S. Frank, D. Schrupp, and M. Scheffler*: A combined DFT/LEED-approach for complex oxide surface structure determination: $\text{Fe}_3\text{O}_4(0\ 0\ 1)$. *Surf. Sci.* **602**, 1299 (2008).
431. *Piccinin, S., C. Stampfl, and M. Scheffler*: First-principles investigation of Ag-Cu alloy surfaces in an oxidizing environment. *Phys. Rev. B* **77**, 075426 (2008).
432. *Richter, M., S. Butscher, N. Bücking, F. Milde, C. Weber, P. Kratzer, M. Scheffler, and A. Knorr*: Theory of ultrafast dynamics of electron-phonon interactions in two dimensional electron gases: Semiconductor quantum wells, surfaces and graphene. In: *Advances in Solid State Physics* **48**. (Ed.) R. Haug. Springer 2008, 281. ISBN 978-3-540-85858-4.
433. *Rinke, P., A. Qteish, J. Neugebauer, and M. Scheffler*: Exciting prospects for solids: Exact-exchange based functionals meet quasiparticle energy calculations. *phys. stat. sol. (b)* **245**, 929 (2008).
434. *Rinke, P., M. Winkelkemper, A. Qteish, D. Bimberg, J. Neugebauer, and M. Scheffler*: Consistent set of band parameters for the group-III nitrides AlN, GaN, and InN. *Phys. Rev. B* **77**, 075202 (2008).
435. *Rogal, J., K. Reuter, and M. Scheffler*: CO oxidation on Pd(100) at technologically relevant pressure conditions: First-principles kinetic Monte Carlo study. *Phys. Rev. B* **77**, 155410 (2008).
436. *Santra, B., A. Michaelides, M. Fuchs, A. Tkatchenko, C. Filippi, and M. Scheffler*: On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters. II. The water hexamer and van der Waals interactions. *J. Chem. Phys.* **129**, 194111 (2008).
437. *Singh, A.K., A. Janotti, M. Scheffler, and C.G. Van de Walle*: Sources of electrical conductivity in SnO_2 . *Phys. Rev. Lett.* **101**, 055502 (2008).
438. *Blum, V., R. Gehrke, F. Hanke, P. Havu, V. Havu, X. Ren, K. Reuter, and M. Scheffler*: Ab initio molecular simulations with numeric atom-centered orbitals. *Comp. Phys. Comm.* **180**, 2175 (2009).
439. *Carlsson, J.M., F. Hanke, S. Linic, and M. Scheffler*: Two-step mechanism for low-temperature oxidation of vacancies in graphene. *Phys. Rev. Lett.* **102**, 166104 (2009).
440. *Carrasco, J., A. Michaelides, and M. Scheffler*: Insight from first principles into the nature of the bonding between water molecules and 4d metal surfaces. *J. Chem. Phys.* **130**, 184707 (2009).
441. *Freysoldt, Ch., P. Rinke, and M. Scheffler*: Controlling polarization at insulating surfaces: Quasiparticle calculations for molecules adsorbed on insulator films. *Phys. Rev. Lett.* **103**, 056803 (2009).

442. *Havu, V., V. Blum, P. Havu, and M. Scheffler*: Efficient $O(N)$ integration for all-electron electronic structure calculation using numeric basis functions. *J. Comp. Phys.* **228**, 8367 (2009).
443. *Hülsen, B., M. Scheffler, and P. Kratzer*: Structural stability and magnetic and electronic properties of $\text{Co}_2\text{MnSi}(001)/\text{MgO}$ heterostructures: A density-functional theory study. *Phys. Rev. Lett.* **103**, 046802 (2009).
444. *Hülsen, B., M. Scheffler, and P. Kratzer*: Thermodynamics of the Heusler alloy $\text{Co}_{2-x}\text{Mn}_{1+x}\text{Si}$: A combined density functional theory and cluster expansion study. *Phys. Rev. B* **79**, 094407 (2009).
445. *Ireta, J. and M. Scheffler*: Density functional theory study of the conformational space of an infinitely long polypeptide chain. *J. Chem. Phys.* **131**, 085104 (2009).
446. *Jiang, H., R.I. Gómez-Abal, P. Rinke, and M. Scheffler*: Localized and itinerant states in lanthanide oxides united by $GW @ \text{LDA} + U$. *Phys. Rev. Lett.* **102**, 126403 (2009).
447. *Kratzer, P., A. Chakrabarti, Q.K.K. Liu, and M. Scheffler*: Theory of shape evolution of InAs quantum dots on $\text{In}_{0.5}\text{Ga}_{0.5}\text{As}/\text{InP}(001)$ substrate. *New J. Phys.* **11**, 073018 (2009).
448. *Meskine, H., S. Matera, M. Scheffler, K. Reuter, and H. Metiu*: Examination of the concept of degree of rate control by first-principles kinetic Monte Carlo simulations. *Surf. Sci.* **603**, 1724 (2009).
449. *Mulakaluri, N., R. Pentcheva, M. Wieland, W. Moritz, and M. Scheffler*: Partial dissociation of water on $\text{Fe}_3\text{O}_4(001)$: Adsorbate induced charge and orbital order. *Phys. Rev. Lett.* **103**, 176102 (2009).
450. *Pentcheva, R., N. Mulakaluri, W.E. Pickett, H.-G. Kleinhenz, W. Moritz, and M. Scheffler*: Compensation mechanisms and functionality of transition metal oxide surfaces and Interfaces: A density functional theory study. In: High Performance Computing in Science and Engineering. (Eds.) S.Wagner, M.Steinmetz, A.Bode, and M.Brehm. Springer Berlin Heidelberg 2009, 709-717. DOI: 10.1007/978-3-540-69182-2.
451. *Piccinin, S., C. Stampfl, and M. Scheffler*: Ag-Cu alloy surfaces in an oxidizing environment: A first-principles study. *Surf. Sci.* **603**, 1467 (2009).
452. *Ren, X., P. Rinke, and M. Scheffler*: Exploring the random phase approximation: Application to CO adsorbed on Cu(111). *Phys. Rev. B* **80**, 045402 (2009).
453. *Richter, M., A. Carmele, S. Butscher, N. Bücking, F. Milde, P. Kratzer, M. Scheffler, and A. Knorr*: Two-dimensional electron gases: Theory of ultrafast dynamics of electron-phonon interactions in graphene, surfaces, and quantum wells. *J. Appl. Phys.* **105**, 122409 (2009).
454. *Rinke, P., A. Janotti, M. Scheffler, and C.G. Van de Walle*: Defect formation energies without the band-gap problem: Combining density-functional theory and the GW approach for the silicon self-interstitial. *Phys. Rev. Lett.* **102**, 026402 (2009).

455. *Santra, B., A. Michaelides, and M. Scheffler*: Coupled cluster benchmarks of water monomers and dimers extracted from density-functional theory liquid water: The importance of monomer deformations. *J. Chem. Phys.* **131**, 124509 (2009).
456. *Schnadt, J., J. Knudsen, X.L. Hu, A. Michaelides, R.T. Vang, K. Reuter, Z. Li, E. Lægsgaard, M. Scheffler, and F. Besenbacher*: Experimental and theoretical study of oxygen adsorption structures on Ag(111). *Phys. Rev. B* **80**, 075424 (2009).
457. *Tkatchenko, A., R.A. DiStasio Jr., M. Head-Gordon, and M. Scheffler*: Dispersion-corrected Møller-Plesset second-order perturbation theory. *J. Chem. Phys.* **131**, 094106 (2009).
458. *Tkatchenko, A. and M. Scheffler*: Accurate molecular van der Waals interactions from ground-state electron density and free-atom reference data. *Phys. Rev. Lett.* **102**, 073005 (2009).
459. *Yan, Q., P. Rinke, M. Scheffler, and C.G. Van de Walle*: Strain effects in group-III nitrides: Deformation potentials for AlN, GaN, and InN. *Appl. Phys. Lett.* **95**, 121111 (2009).
460. *Hashemifar, S.J., P. Kratzer, and M. Scheffler*: Stable structure and magnetic state of ultrathin CrAs films on GaAs(001): A density functional theory study. *Phys. Rev. B* **82**, Issue 21 (2010).
461. *Havu, P., V. Blum, V. Havu, P. Rinke, and M. Scheffler*: Large-scale surface reconstruction energetics of Pt(100) and Au(100) by all-electron density functional theory. *Phys. Rev. B* **82**, 161418(R) (2010).
462. *Jiang, H., R.I. Gomez-Abal, P. Rinke, and M. Scheffler*: Electronic band structure of zirconia and hafnia polymorphs from the *GW* perspective. *Phys. Rev. B* **81**, 085119 (2010).
463. *Jiang, H., R.I. Gomez-Abal, P. Rinke, and M. Scheffler*: First-principles modeling of localized *d* states with the *GW@LDA+U* approach. *Phys. Rev. B* **82**, 045108 (2010).
464. *Marom, N., A. Tkatchenko, M. Scheffler, and L. Kronik*: Describing both dispersion interactions and electronic structure using density functional theory: The case of metal-phthalocyanine dimers. *J. Chem. Theory Comput.* **6**, 81 (2010).
465. *Michaelides, A. and M. Scheffler*: An introduction to the theory of metal surfaces. To appear in: *Textbook of Surface and Interface Science*, Vol. I. (Ed.) K. Wandelt, Wiley-VCH (2010).
466. *Mulakaluri, N., R. Pentcheva, and M. Scheffler*: Coverage-dependent adsorption mode of water on Fe₃O₄(001): Insights from first principles calculations. *J. Phys. Chem. C* **114**, 11148 (2010).

467. *Myrach, P., N. Nilius, S. Levchenko, A. Gonchar, T. Risse, K.-P. Dinse, L.A. Boatner, W. Frandsen, R. Horn, H.-J. Freund, R. Schlögl, and M. Scheffler:* Temperature-dependent morphology, magnetic, and optical properties of Li-doped MgO. *ChemCatChem* **2**, 854 (2010).
468. *Piccinin, S., N.L. Nguyen, C. Stampfl, and M. Scheffler:* First-principles study of the mechanism of ethylene epoxidation over Ag-Cu particles. *J. Mater. Chem.* **20**, 10521 (2010).
469. *Piccinin, S., S. Zafeiratos, C. Stampfl, T.W. Hansen, M. Hävecker, D. Teschner, V.I. Bukhtiyarov, F. Girgsdies, A. Knop-Gericke, R. Schlögl, and M. Scheffler:* Alloy catalyst in a reactive environment: The example of Ag-Cu particles for ethylene epoxidation. *Phys. Rev. Lett.* **104**, 035503 (2010).
470. *Rossi, M., V. Blum, P. Kupser, G. von Helden, F. Bierau, K. Pagel, G. Meijer, and M. Scheffler:* Secondary Structure of Ac-Ala_n-LysH⁺ Polyalanine Peptides ($n=5, 10, 15$) in Vacuo: Helical or Not?. *J. Phys. Chem. Lett.* **1**, 3465 (2010).
471. *Tkatchenko, A., L. Romaner, O.T. Hofmann, E. Zojer, C. Ambrosch-Draxl, and M. Scheffler:* Van der Waals interactions between organic adsorbates and at organic/inorganic interfaces. *MRS Bulletin* **35**, 435 (2010).
472. *Wu, H., A. Stroppa, S. Sakong, S. Picozzi, M. Scheffler, and P. Kratzer:* Magnetism in C or N-doped MgO and ZnO: A Density-Functional Study of Impurity Pairs. *Phys. Rev. Lett.* **105**, 267203 (2010).
473. *Yan, Q., P. Rinke, M. Scheffler, and C.G. Van de Walle:* Role of strain in polarization switching in semipolar InGaN/GaN quantum wells. *Appl. Phys. Lett.* **97**, 181102 (2010).
474. *Arndt, S., G. Laugel, S. Levchenko, R. Horn, M. Baerns, M. Scheffler, R. Schlögl, and R. Schomäcker:* A Critical Assessment of Li/MgO-Based Catalysts for the Oxidative Coupling of Methane. *Catal. Rev. Sci. Eng.* **53**, 424 (2011).
475. *Beret, E.C., L.M. Ghiringhelli, and M. Scheffler:* Free gold clusters: Beyond the static, mono-structure description. *Faraday Discuss.*, **152 (1)**, 153 (2011).
476. *Estreicher, S.K., D.J. Backlund, C. Carbogno, and M. Scheffler:* Activation Energies for Diffusion of Defects in Si: The Role of the Exchange-Correlation Functional. *Angew. Chem.*, **123**, 1 (2011).
477. *Fichthorn, K.A., Y. Tiwary, T. Hammerschmidt, P. Kratzer, and M. Scheffler:* Analytic many-body potential for GaAs(001) homoepitaxy: Bulk and surface properties. *Phys. Rev. B* **83**, 195328 (2011).
478. *Freund, H., G. Meijer, M. Scheffler, R. Schlögl, and M. Wolf:* CO oxidation as a prototypical reaction for heterogeneous processes. *Angew. Chem. Int.* **50**, 10064 (2011).

479. *Marom, N., A. Tkatchenko, M. Rossi, V.V. Gobre, O. Hod, M. Scheffler, and L. Kronik*: Dispersion interactions with density-functional theory: Benchmarking semi-empirical and inter-atomic pair-wise corrected density functionals. *J. Chem. Theory Comput.* **7** 3944 (2011).
480. *Ren, X., A. Tkatchenko, P. Rinke, and M. Scheffler*: Beyond the random-phase approximation for the electron correlation energy: The importance of single excitations. *Phys. Rev. Lett.* **106**, 153003 (2011).
481. *Santra, B., J. Klimeš, D. Alfè, A. Tkatchenko, B. Slater, A. Michelides, R. Car, and M. Scheffler*: Hydrogen bonds and van der Waals forces in ice at ambient and high pressures. *Phys. Rev. Lett.* **107**, 185701 (2011).
482. *Tkatchenko, A., M. Rossi, V. Blum, J. Ireta, and M. Scheffler*: Unraveling the stability of polypeptide helices: Critical role of van der Waals interactions. *Phys. Rev. Lett.*, **106**, 118102 (2011).
483. *Yan, Q., P. Rinke, M. Winkelkemper, A. Qteish, D. Bimberg, M. Scheffler, and C.G. Van de Walle*: Band parameters and strain effects in ZnO and group-III nitrides. *Semicond. Sci. Technol.*, **26**, 014037 (2011).
484. *Yoon, M., Y. Miyamoto, and M. Scheffler*: Enhanced dipole moments in photo-excited TTF-TCNQ dimers. *New J. Phys.* **13**, 073039 (2011).
485. *Zhang, G.X., A. Tkatchenko, J. Paier, H. Appel, and M. Scheffler*: Van der Waals interactions in ionic and semiconductor solids. *Phys. Rev. Lett.* **107**, 245501 (2011).
486. *Caruso, F., P. Rinke, X. Ren, M. Scheffler and A. Rubio*: Unified description of ground and excited states of finite systems: the self-consistent *GW* approach. *Phys. Rev. B* **86**, 081102(R) (2012).
487. *Casadei, M., X. Ren, P. Rinke, A. Rubio, and M. Scheffler*: Density-functional Theory for *f*-electron Systems: the α - γ Phase Transition in Cerium. *Phys. Rev. Lett.* **109**, 146402 (2012).
488. *Jiang, H., R.I. Gómez-Abal, X.-Z. Li, C. Meisenbichler, C. Ambrosch-Draxl, and Matthias Scheffler*: FHI-gap: A *GW* code based on the all-electron augmented plane wave method. *Comp. Phys. Com.* **184**, 348 (2012).
489. *Jiang, H., P. Rinke, and M. Scheffler*: Electronic properties of lanthanide oxides from the *GW* perspective. *Phys. Rev. B* **86**, 125115 (2012).
490. *Kim, H.-J., A. Tkatchenko, J.-H. Cho, and M. Scheffler*: Benzene Adsorbed on Si(001): The Role of Electron Correlation and Finite Temperature. *Phys. Rev. B* **85** (R), 041403 (2012).
491. *Li, X.Z., R. Gómez-Abal, H. Jiang, C. Ambrosch-Draxl, and M. Scheffler*: Impact of widely used approximations to the G0W0 method: An all-electron perspective. *New J. Phys.* **14**, 023006 (2012).

492. *Liu, W., A. Savara, X. Ren, W. Ludwig, K.-H. Dostert, S. Schauermann, A. Tkatchenko, H.-J. Freund, and M. Scheffler*: Toward Low-Temperature Dehydrogenation Catalysis: Isophorone Adsorbed on Pd(111). *J. Phys. Chem. Lett.* **3**, 582 (2012).
493. *Liu, W., J. Carrasco, B. Santra, A. Michaelides, M. Scheffler, and A. Tkatchenko*: Benzene Adsorbed on Metals: Concerted Effect of Covalency and van der Waals Bonding. *Phys. Rev. B* **86**, 245405 (2012).
494. *Marom, N., F. Caruso, X. Ren, O. Hofmann, T. Körzdörfer, J. R. Chelikowsky, A. Rubio, M. Scheffler, and P. Rinke*: Benchmark of GW Methods for Azabenzenes. *Phys. Rev. B* **86**, 245127 (2012).
495. *Michaelides, A. and M. Scheffler*: An introduction to the theory of crystalline elemental solids and their surfaces. In *Surface and Interface Science*, ISBN 978-3-527-41156-6, edited by K. Wandelt, 13 (2012).
496. *Paier, J., X. Ren, P. Rinke, G.E. Scuseria, A. Grüneis, G. Kresse, and M. Scheffler*: Assessment of correlation energies based on the random-phase approximation. *New J. Phys.* **14**, 043002 (2012).
497. *Ramprasad, R., H. Zhu, P. Rinke, and M. Scheffler*: New perspective on formation energies and energy levels of point defects in non-metals. *Phys. Rev. Lett.* **108**, 0666404 (2012).
498. *Ren, X., P. Rinke, V. Blum, J. Wieferink, A. Tkatchenko, A. Sanfilippo, K. Reuter, and M. Scheffler*: Resolution-of-identity approach to Hartree-Fock, hybrid density functionals, RPA, MP2, and GW with numeric atom-centered orbital basis functions. *New J. Phys.* **14**, 053020 (2012).
499. *Ren, X., P. Rinke, C. Joas, and M. Scheffler*: Invited Review: Random-phase approximation and its applications in computational chemistry and materials science. *J. Mater. Sci.* **47**, 7447 (2012).
500. *Rinke, P., A. Schleife, E. Kioupakis, A. Janotti, C. Rödl, F. Bechstedt, M. Scheffler, and C.G. Van de Walle*: First-principles optical spectra of F centers in MgO. *Phys. Rev. Lett.* **108**, 126404 (2012).
501. *Ruiz, V.G., W. Liu, E. Zojer, M. Scheffler, and A. Tkatchenko*: Density-functional theory with screened van der Waals interactions for the modeling of hybrid inorganic/organic systems. *Phys. Rev. Lett.* **108**, 146103 (2012).
502. *Tkatchenko, A., R.A. DiStasio, Jr., R. Car, and M. Scheffler*: Accurate and efficient method for many-body van der Waals interactions. *Phys. Rev. Lett.* **108**, 236402 (2012).
503. *Yan, Q., A. Janotti, M. Scheffler, and C.G. Van de Walle*: Role of nitrogen vacancies in the luminescence of Mg-doped GaN. *Appl. Phys. Lett.* **100**, 142110 (2012).

504. Yan, Q., P. Rinke, M. Winkelnkemper, A. Qteish, D. Bimberg, M. Scheffler, and C.G. Van de Walle: Strain effects and band parameters in MgO, ZnO, and CdO. *Appl. Phys. Lett.* **101**, 152105 (2012).
505. Atalla, V., M. Yoon, F. Caruso, P. Rinke, and M. Scheffler: Hybrid density functional theory meets quasiparticle calculations: A consistent electronic structure approach. *Phys. Rev. B* **88**, 165122 (2013).
506. Baldauf, C., K. Pagel, S. Warnke, G. von Helden, B. Koksch, V. Blum, and M. Scheffler: How Cations Change Peptide Structure. Accepted to *Chem. - A European J.* (May 15, 2013).
507. Bhattacharya, S., S.V. Levchenko, L.M. Ghiringhelli, and M. Scheffler: Stability and metastability of clusters in a reactive atmosphere: theoretical evidence for unexpected stoichiometries of $Mg_M O_x$. *Phys. Rev. Lett.* **111**, 135501 (2013).
508. Caruso, F., D.R. Rohr, M. Hellgren, X. Ren, P. Rinke, A. Rubio, and M. Scheffler: Bond Breaking and Bond Formation: How Electron Correlation is Captured in Many-Body Perturbation Theory and Density-Functional Theory. *Phys. Rev. Lett.* **110**, 146403 (2013).
509. Caruso F., P. Rinke, X. Ren, A. Rubio, and M. Scheffler: Self-consistent GW : an all-electron implementation with localized basis functions. *Phys. Rev. B* **88**, 075105 (2013).
510. Ghiringhelli, L.M., P. Gruene, J.T. Lyon, D.M. Rayner, G. Meijer, A. Fielicke, and M. Scheffler: Not so loosely bound rare gas atoms: finite-temperature vibrational fingerprints of neutral gold-cluster complexes. *New J. Phys.* **15**, 083003 (2013) .
511. Hansen, K., G. Montavon, F. Biegler, S. Fazli, M. Rupp, M. Scheffler, O.A. von Lilienfeld, A. Tkatchenko, and K.-R. Müller: Assessment and Validation of Machine Learning Methods for Predicting Molecular Atomization Energies. *J. Chem. Theory Comput.* **9**, 3404-3419 (2013).
512. Hofmann, O.T., J.C. Deinert, Y. Xu, P. Rinke, J. Stähler, M. Wolf, and M. Scheffler: Large work function reduction by adsorption of a molecule with a negative electron affinity: Pyridine on ZnO(1010). *J. Chem. Phys.* **139**, 174701 (2013).
513. Hofmann, O.T., N. Moll, P. Rinke, and M. Scheffler: Interface dipoles of organic molecules on Ag(111) in hybrid density-funktional theory. *New J. Phys.* **15**, 123028 (2013).
514. Kendelewicz, T., S. Kaya, J.T. Newberg, H. Blum, N. Mulakaluri, W. Moritz, M. Scheffler A. Nilsson, R. Pentcheva, and G.E. Brown, Jr.: X-ray Photoemission and Density Functional Theory Study of the Interaction of Water Vapor with $Fe_3O_4(001)$ Surface at Near-Ambient Conditions. *J. Phys. Chem. C* **117**, 2719 (2013).

515. *Liu, W., V.G. Ruiz, G.-X. Zhang, B. Santra, X. Ren, M. Scheffler, and A. Tkatchenko*: Structure and energetics of benzene adsorbed on transition-metal surfaces: Density-functional theory with van der Waals interactions including collective substrate response. *New J. Phys.* **15**, 053043 (2013).
516. *Nemec, L., V. Blum, P. Rinke, and M. Scheffler*: Thermodynamic equilibrium conditions of graphene films on SiC. *Phys. Rev. Lett.* **111**, 065502 (2013).
517. *Ren, X., P. Rinke, G.E. Scuseria, and M. Scheffler*: Renormalized Second-order Perturbation Theory for The Electron Correlation Energy: Concept, Implementation, and Benchmarks. *Phys. Rev. B* **88**, 035120 (2013).
518. *Richter, N.A., S. Sicolo, S.V. Levchenko, J. Sauer, and M. Scheffler*: Concentration of Vacancies at Metal Oxide Surfaces: Case Study of MgO (100). *Phys. Rev. Lett.* **111**, 045502 (2013).
519. *Rossi, M., M. Scheffler, and V. Blum*: Impact of Vibrational Entropy on the Stability of Unsolvated Peptide Helices with Increasing Length. *J. Phys. Chem. B* **117** (18), 5574-5584 (2013).
520. *Santra, B., J. Klimes, A. Tkatchenko, D. Alfè, B. Slater, A. Michaelides, R. Car, and M. Scheffler*: On the Accuracy of van der Waals Inclusive Density-Functional Theory Exchange-Correlation Functionals for Ice at Ambient and High Pressures. *J. Chem. Phys.* **139**, 154702 (2013).
521. *Schlesinger, R., Y. Xu, O.T. Hofmann, S. Winkler, J. Frisch, J. Niederhausen, A. Vollmer, S. Blumstengel, F. Henneberger, P. Rinke, M. Scheffler, and N. Koch*: Controlling the work function of ZnO and the energy-level alignment at the interface to organic semiconductors with a molecular electron acceptor. *Phys. Rev. B* **87**, 155311 (2013).
522. *Schumann, T., M. Dubslaff, M.H. Oliveira Jr, M. Hanke, F. Fromm, T. Seyller, L. Nemec, V. Blum, M. Scheffler, J.M.J. Lopes, and H. Riechert*: Structural investigation of nanocrystalline graphene grown on $(6\sqrt{3}\times 6\sqrt{3})$ R30°-reconstructed SiC surfaces by molecular beam epitaxy. *New J. Phys.* **15**, 123034 (2013).
523. *Yu, J., M. Scheffler, and H. Metiu*: Oxidative Dehydrogenation of Methane by Isolated Vanadium Oxide Clusters Supported on Au (111) and Ag (111) Surfaces. *J. Phys. Chem. C* **117**, 18475-18483 (2013).
524. *Xu, Y., O.T. Hofmann, R. Schlesinger, S. Winkler, J. Frisch, J. Niederhausen, A. Vollmer, S. Blumstengel, F. Henneberger, N. Koch, P. Rinke, and M. Scheffler*: Space Charge Transfer in Hybrid Inorganic-Organic Systems. *Phys. Rev. Lett.* **111**, 226802 (2013).
525. *Zhang, I.Y., X. Ren, P. Rinke, V. Blum, and M. Scheffler*: Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. *New J. Phys.* **15**, 123033 (2013).

526. *Bhattacharya, S., S. Levchenko, L.M. Ghiringhelli and M. Scheffler*: Efficient *ab initio* schemes for finding thermodynamically stable and metastable atomic structures: Benchmark of cascade genetic algorithms. *New J. Phys.* **16**, 123016 (2014).
527. *Carbogno, Ch., C.G. Levi, C.G. Van de Walle, and M. Scheffler*: Ferroelastic switching of doped zirconia: Modeling and understanding from first principles. *Phys. Rev. B* **90**, 144109 (2014).
528. *Caruso, F., V. Atalla, X. Ren, A. Rubio, M. Scheffler, and P. Rinke*: First-Principles Description of Charge Transfer in Donor-Acceptor Compounds from Self-Consistent Many-Body Perturbation Theory. *Phys. Rev. B* **90**, 085141 (2014).
529. *Liu, W., A. Tkatchenko, and M. Scheffler*: Modeling Adsorption and Reactions of Organic Molecules at Metal Surfaces. *Acc. Chem. Res.* **47**, 3369-3377 (2014).
530. *Rossi, M., S. Chutia, M. Scheffler, and V. Blum*: Validation Challenge of Density-Functional Theory for Peptides - Example of Ac-Phe-Ala₅-LysH⁺. *J. Phys. Chem. A* **118** (35), 7349-7359 (2014).
531. *Yan, Q., A. Janotti, M. Scheffler, and Ch.G. Van de Walle*: Origins of optical absorption and emission lines in AlN. *Appl. Phys. Lett.* **105**, 111104 (2014).
532. *Yan, Q., P. Rinke, A. Janotti, M. Scheffler, and Ch. G. Van de Walle*: Effects of strain on the band structure of group-III nitrides. *Phys. Rev. B* **90**, 125118 (2014).
533. *Ghiringhelli, L.M., J. Vybiral, S.V. Levchenko, C. Draxl, and M. Scheffler*: Big Data of Materials Science - Critical Role of the Descriptor. *Phys. Rev. Lett.* **114**, 105503 (2015).
534. *Hellgren, M., F. Caruso, D.R. Rohr, X. Ren, A. Rubio, M. Scheffler, and P. Rinke*: Static correlation and electron localization in molecular dimers from the self-consistent RPA and GW approximation. *Phys. Rev. B* **91**, 165110 (2015).
535. *Hoffmann, M.J., M. Scheffler, and K. Reuter*: Multi-lattice Kinetic Monte Carlo Simulations from First Principles: Reduction of the Pd(100) Surface Oxide by CO. *ACS Catalysis* **5**, 1199-1209 (2015).
536. *Hofmann, O.T., P. Rinke, M. Scheffler, and G. Heimel*: Integer versus Fractional Charge Transfer at Metal(/Insulator)/Organic Interfaces: Cu(/NaCl)/TCNE. *ACS Nano* **9**, 5391-5404 (2015).
537. *Ihrig, A.C., J. Wieferink, I.Y. Zhang, M. Ropo, X. Ren, P. Rinke, M. Scheffler, and V. Blum*: Accurate localized resolution of identity approach for linear-scaling hybrid density functionals and for many-body perturbation theory. *New J. Phys.* **17**, 093020 (2015).
538. *Knuth, F. , C. Carbogno, V. Atalla, V. Blum, and M. Scheffler*: All-electron Formalism for Total Energy Strain Derivatives and Stress Tensor Components for Numeric Atom-Centered Orbitals. *Comp. Phys. Comm.* **190**, 33-50 (2015).

539. *Levchenko, S.V., X. Ren, J. Wieferink, P. Rinke, V. Blum, M. Scheffler, and R. Johann:* Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. *Comp. Phys. Comm.* **192**, 60-69 (2015).
540. *Nemeč, L., F. Lazarević, P. Rinke, M. Scheffler, and V. Blum:* Why graphene growth is very different on the C face than on the Si face of SiC: Insights from surface equilibria and the (3x3)-3C-SiC(111) reconstruction. *Phys. Rev. B* **91**, 161408(R) (2015).
541. *Pinheiro Jr., M., M.J. Caldas, P. Rinke, V. Blum, and M. Scheffler:* Length Dependence of Ionization Potentials of Trans-Acetylenes: Internally-Consistent DFT/GW Approach. *Phys. Rev. B* **92**, 195134 (2015).
542. *Richter, N.A., F. Stavale, S.V. Levchenko, N. Nilius, H.-J. Freund, and M. Scheffler:* Defect complexes in Li-doped MgO. *Phys. Rev. B* **91**, 195305 (2015).
543. *Ren, X., N. Marom, F. Caruso, M. Scheffler, and P. Rinke:* Beyond the GW approximation: A second-order screened exchange correction. *Phys. Rev. B* **92**, 081104 (2015).
544. *Ruzsinszky, A. , I.Y. Zhang, and M. Scheffler:* Insight into organic reactions from the direct random phase approximation and its corrections. *J. Chem. Phys.* **143**, 144115 (2015).
545. *Schubert, F., K. Pagel, M. Rossi, S. Warnke, M. Salwiczek, B. Koksich, G. von Helden, V. Blum, C. Baldauf, and M. Scheffler:* Native like helices in a specially designed b peptide in the gas phase. *Phys. Chem. Chem. Phys.* **17**, 5376 (2015).
546. *Schubert, F. , M. Rossi, C. Baldauf, K. Pagel, S. Warnke, G. von Helden, F. Filsinger, P. Kupser, G. Meijer, M. Salwiczek, B. Koksich, M. Scheffler, and V. Blum:* Exploring the conformational preferences of 20-residue peptides in isolation: Ac-Ala19-Lys + H+ vs. Ac-Lys-Ala19 + H+ and the current reach of DFT. *Phys. Chem. Chem. Phys.* **17**, 7373-7385 (2015).
547. *Sezen, H., H. Shang, F. Bebensee, C. Yang, M. Buchholz, A. Nefedov, S. Heissler, Ch. Carbogno, M. Scheffler, P. Rinke, and Ch. Wöll:* Evidence for photogenerated intermediate hole polarons in ZnO. *Nat. Comm.* **6**, 6901 (2015).
548. *Sinai, O., O.T. Hofmann, P. Rinke, M. Scheffler, G. Heimel, and L. Kronik:* Multiscale approach to the electronic structure of doped semiconductor surfaces. *Phys. Rev.B* **91**, 075311 (2015).
549. *van Setten, M.J., F. Caruso, S. Sharifzadeh, X. Ren, M. Scheffler, F. Liu, J. Lischner, L. Lin, J.R. Deslippe, S.G. Louie, C. Yang, F. Weigend, J.B. Neaton, F. Evers, and P. Rinke:* GW 100: Benchmarking G_0W_0 for molecular systems. *J. Chem. Theory Comput.* **11**, 5665-5687 (2015).
550. *Atalla, V., I.Y. Zhang, O.T. Hofmann, X. Ren, P. Rinke, and M. Scheffler:* Enforcing the linear behavior of the total energy with hybrid functionals: Implications for charge transfer, interaction energies, and the random-phase approximation. *Phys. Rev. B* **94**, 035140 (2016).

551. *Casadei, M., X. Ren, P. Rinke, A. Rubio, and M. Scheffler*: Density functional theory study of the - phase transition in cerium: Role of electron correlation and f-orbital localization. *Phys. Rev. B* **93**, 075153 (2016).
552. *Chibani, W., X. Ren, M. Scheffler, and P. Rinke*: Self-Consistent Green's Function Embedding for Advanced Electronic Structure Methods Based on a Dynamical Mean-Field Concept. *Phys. Rev. B* **93**, 165106 (2016).
553. *Ghiringhelli, L.M., C. Carbogno, S. Levchenko, F. Mohamed, G. Huhs, M. Lueders, M. Oliveira, and M. Scheffler*: Towards a Common Format for Computational Materials Science Data. Published as "k Scientific Highlight of the Month", n. 131 (July 2016).
554. *Lejaeghere, K., G. Bihlmayer, T. Bjrkman et al.*: Reproducibility in density functional theory calculations of solids. *Science* **351**, aad3000 (2016).
555. *Nieminen, R.M., S. Bonella, L. Drury, M. Scheffler, and E. Molinari*: Three European Centers of Excellence in Computational Science. *Psi_k Scientific Highlight Of The Month*, **133** (2016).
556. *Scheffler, M. and D. Hoffmann*: Obituary: Walter Kohn (1923-2016). *Nat. Mater.* **15**, 704 (2016).
557. *Scheffler, M. and D. Hoffmann*: Zum Gedenken an Walter Kohn. *Phys. J.* **15**, 7 (2016).
558. *Schwarz, K., L.J. Sham, A.E. Mattsson, and M. Scheffler*: Obituary for Walter Kohn (1923-2016). *Computation* **4**, 40 (2016).
559. *Zhang, I.Y., P. Rinke, J.P. Perdew, and M. Scheffler*: Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. *Phys. Rev. Lett.* **117**, 133002 (2016).
560. *Zhang, I.Y., P. Rinke, and M. Scheffler*: Wave-function inspired density functional applied to the H₂/H₂⁺ challenge. *New J. Phys.* **18**, 073026 (2016).
561. *Bhattacharya, A., C. Carbogno, B. Bhme, M. Baitinger, Y. Grin, and M. Scheffler*: Formation of Vacancies in Si- and Ge-based Clathrates: Role of Electron Localization and Symmetry Breaking. *Phys. Rev. Lett.* **118**, 236401 (2017).
562. *Carbogno, C., R. Ramprasad, and M. Scheffler*: *Ab initio* Green-Kubo Approach for the Thermal Conductivity of Solids. *Phys. Rev. Lett.* **118**, 175901 (2017).
563. *Draxl, C., F. Illas, and M. Scheffler*: Computational materials: Open data settled in materials theory. *Nat.* **548**, 523 (2017).
564. *Ghiringhelli, L.M., C. Carbogno, S.V. Levchenko, F. Mohamed, G. Huhs, M. Lueders, M. Oliveira, and M. Scheffler*: Towards efficient data exchange and sharing for big-data driven materials science: metadata and data formats. *npj Computational Materials* **3**, 46 (2017).

565. *Ghiringhelli, L.M., J. Vybiral, E. Ahmetcik, R. Ouyang, S.V. Levchenko, C. Draxl, and M. Scheffler*: Learning physical descriptors for materials science by compressed sensing. *New J. Phys.* **19**, 023017 (2017).
566. *Goldsmith, B.R., M. Boley, J. Vreeken, M. Scheffler, and L.M. Ghiringhelli*: Uncovering structure-property relationships of materials by subgroup discovery. *New J. Phys.* **19**, 013031 (2017).
567. *Perdew, J.P., W. Yang, K. Burke, Z. Yang, E.K.U. Gross, M. Scheffler, et al.*: Understanding Band Gaps of Solids in Generalized Kohn-Sham Theory. *PNAS* **114**, 11 (2017).
568. *Shang, H., C. Carbogno, P. Rinke, and M. Scheffler*: Lattice Dynamics Calculations based on Density-functional Perturbation Theory in Real Space. *Comp. Phys. Comm.* **215**, 26-46 (2017).
569. *Ziletti, A., D. Kumar, M. Scheffler, and L.M. Ghiringhelli*: The face of crystals: insightful classification using deep learning. Submitted to *Nat. Commun.* (September 7, 2017).
570. *Draxl, C. and M. Scheffler*: NOMAD: The FAIR Concept for Big-Data-Driven Materials Science. Invited Review for *MRS Bulletin* **43**, 676-682 (2018).
571. *Kokott, S., S.V. Levchenko, P. Rinke, and M. Scheffler*: First-principles supercell calculations of small polarons with proper account for long-range polarization effects. *New J. Phys.* **20**, 033023 (2018).
572. *Oses, C., E. Gossett, D. Hicks, F. Rose, M.J. Mehl, E. Perim, I. Takeuchi, S. Sanvito, M. Scheffler, Y. Lederer, O. Levy, C. Toher, and S. Curtarolo*: AFLOW-CHULL: Cloud-Oriented Platform for Autonomous Phase Stability Analysis. Published in *J. Chem. Inf. Model* (September 6, 2018).
573. *Ouyang, R., S. Curtarolo, E. Ahmetcik, M. Scheffler, and L.M. Ghiringhelli*: SISSO: a compressed-sensing method for identifying the best low-dimensional descriptor in an immensity of offered candidates . *Phys. Rev. Mat.* **2**, 083802 (2018).
574. *Rasim, K., R. Ramlau, A. Leithe-Jasper, T. Mori, U. Burkhardt, H. Borrmann, W. Schnelle, C. Carbogno, M. Scheffler, and Y. Grin*: Local Atomic Arrangements and Band Structure of Boron Carbide. *Angew. Chem.* **57**, 6130-6135 (2018).
575. *Scheffler, M. and Draxl, D.*: Ein FAIRes Datenkonzept der von Big Data gesteuerten Materialwissenschaften. *Jahrbuch / Max-Planck-Gesellschaft* (2018).
576. *Shang, H., N. Raimbault, P. Rinke, M. Scheffler, M. Rossi, and C. Carbogno*: All-Electron, Real-Space Perturbation Theory for Homogeneous Electric Fields: Theory, Implementation, and Application within DFT. *New J. Phys.* **20**, 073040 (2018).

577. *Zhang, G.-X., A. Reilly, A. Tkatchenko, and M. Scheffler*: Performance of various density-functional approximations for cohesive properties of 64 bulk solids. *New J. of Phys.* **20**, 063020 (2018).
578. *Acosta, C.M., R. Ouyang, A. Fazzio, M. Scheffler, L.M. Ghiringhelli, and C. Carbogno*: Analysis of Topological Transitions in Two-dimensional Materials by Compressed Sensing. Submitted to *Nature Materials* (May 28, 2018).
579. *Alvermann, A., A. Basermann, H.-J. Bungartz, C. Carbogno, D. Ernst, H. Fehske, Y. Futamura, M. Galgon, G. Hager, S. Huber, T. Huckle, A. Ida, A. Imakura, M. Kawai, S. Köcher, M. Kreutzer, P. Kus, B. Lang, H. Lederer, V. Manin, A. Marek, K. Nakajima, L. Nemec, K. Reuter, M. Rippl, M. Röhrig-Zöllner, T. Sakurai, M. Scheffler, C. Scheurer, F. Shahzad, D. Simoes Brambila, J. Thies, and G. Wellein*: Benefits from using mixed precision computations in the ELPA-AEO and ESSEX-II eigensolver projects. *Japan J. Indust. Appl. Math.* **36**, 699-717 (2019).
580. *Andersen, M., S.V. Levchenko, M. Scheffler, and K. Reuter*: Beyond Scaling Relations for the Description of Catalytic Materials. *ACS Catal.* **9**, 2752-2759 (2019).
581. *Bartel, C.J., C. Sutton, B.R. Goldsmith, R. Ouyang, C.B. Musgrave, L.M. Ghiringhelli, and M. Scheffler*: New Tolerance Factor to Predict the Stability of Perovskite Oxides and Halides. *Sci. Adv.* **5**, eaav0693 (2019).
582. *Draxl, C. and M. Scheffler*: Big-Data-Driven Materials Science and its FAIR Data Infrastructure. Plenary Chapter in Handdbook of Materials Modeling (eds. S. Yip and W. Andreoni), Springer (2018).
583. *Draxl, C. and M. Scheffler*: The NOMAD Laboratory: From Data Sharing to Artificial Intelligence. *J. Phys. Mater.* **2**, 036001 (2019).
584. *Goldsmith, B.R., J. Florian, J.-X. Liu, Ph. Gruene, J.T. Lyon, D.M. Rayner, A. Fielicke, M. Scheffler, and L.M. Ghiringhelli*: Two-to-three dimensional transition in neutral gold clusters: The crucial role of van der Waals interactions and temperature. *Phys. Rev. Mat.* **3**, 016002 (2019).
585. *Kus, P., A. Marek, S.S. Kcher, H.-H. Kowalski, C. Carbogno, Ch. Scheurer, K. Reuter, M. Scheffler, and H. Lederer*: Optimizations of the Eigensolvers in the ELPA Library. *Parallel Computing* **85**, 167 (2019).
586. *Lenz, M.-O., T.A.R. Purcell, D. Hicks, S. Curtarolo, M. Scheffler, C. Carbogno*: Parametrically constrained geometry relaxations for high-throughput materials science. *npj Computational Materials* **5**, 123 (2019).
587. *Levchenko, S.V. and M. Scheffler*: Compact representation of one-particle wavefunctions and scalar fields obtained from electronic-structure calculations. *Comput. Phys. Comm.* **237**, 42-46 (2019).
588. *Nørskov, J.K., et al.*: Research needs towards sustainable production of fuels and chemicals. (2019).

589. *Ouyang, R., E. Ahmetcik, C. Carbogno, M. Scheffler, and L. M. Ghiringhelli*: Simultaneous Learning of Several Materials Properties from Incomplete Databases with Multi-Task SISSO. *J. Phys. Mater.* **2**, 024002 (2019).
590. *Schewski, R., K. Lion, A. Fiedler, C. Wouters, A. Popp, S.V. Levchenko, T. Schulz, M. Schmidbauer, S. Bin Anooz, R. Grneberg, Z. Galazka, G. Wagner, K. Irmscher, M. Scheffler, C. Draxl, and M. Albrecht*: Step-flow growth in homoepitaxy of - Ga_2O_3 (100)The influence of the miscut direction and faceting. *APL Materials* **7**, 022515 (2019).
591. *Schunk, S.A., et al.*: The Digitalization of Catalysis-Related Sciences. GeCatS Whitepaper (March 2019).
592. *Shang, H., A. Argondizzo, S. Tan, J. Zhao, P. Rinke, C. Carbogno, M. Scheffler, and H. Petek*: Electron-phonon coupling in d-electron solids: A temperature-dependent study of rutile TiO_2 by first-principles theory and two-photon photoemission. *Phys. Rev. Research* **1**, 033153 (2019).
593. *Sutton, C., L.M. Ghiringhelli, T. Yamamoto, Y. Lysogorskiy, L. Blumenthal, T. Hammerschmidt, J. Golebiowski, X. Liu, A. Ziletti, and M. Scheffler*: Crowd-sourcing materials-science challenges with the NOMAD 2018 Kaggle competition. *npj Computational Materials* **5**, 111 (2019).
594. *Wang, H., S.V. Levchenko, T. Schultz, N. Koch, M. Scheffler, and M. Rossi*: Critical Interplay of Atomic and Electronic Structures at Organic/Inorganic Interfaces: The Examples of F4-TCNQ and F6-TCNNQ on H-Si(111). Submitted to *Adv. Mater.* (Oct 31, 2018).
595. *Zhang, I.-Y., A.J. Logsdail, X. Ren, S.V. Levchenko, L. Ghiringhelli, and M. Scheffler*: Main-group test set for materials science and engineering with user-friendly graphical tools for error analysis: Systematic benchmark of the numerical and intrinsic errors in state-of-the-art electronic-structure approximations. *New J. Phys.* **1**, 013025 (2019).
596. *Zhou, Y., M. Scheffler, and L.M. Ghiringhelli*: Determining Surface Phase Diagrams Including Anharmonic Effects. *Phys. Rev. B* **100**, 174106B (2019).
597. *Cao, G., R. Ouyang, L.M. Ghiringhelli, M. Scheffler, H. Liu, C. Carbogno, and Z. Zhang*: Artificial Intelligence for High-Throughput Discovery of Topological Insulators: The Example of Alloyed Tetradymites. *Phys. Rev. Materials* **4**, 034204 (2020).
598. *Janke, S.M., M. Rossi, S.V. Levchenko, S. Kokott, M. Scheffler, and V. Blum*: Pentacene and Tetracene Molecules and Films on H/Si(111): Level Alignment from Hybrid Density Functional Theory. Submitted to *Electron. Struct.* (April 13, 2020).
599. *Knoop, F., T.A.R. Purcell, M. Scheffler, and C. Carbogno*: Anharmonicity Measure for Materials. Submitted to *Phys. Rev. Materials* (June 25, 2020).

600. *Mazheika, A., Y. Wang, R. Valero, L.M. Ghiringhelli, F. Vies, F. Illas, S. V. Levchenko, and M. Scheffler: Ab initio data-analytics study of carbon-dioxide activation on semiconductor oxide surfaces.* Submitted to ACS catalysis (Dec 13, 2019).
601. *Ren, X., F. Merz, H. Jiang, Y. Yao, M. Rampp, H. Lederer, V. Blum, and M. Scheffler: All-electron periodic G_0W_0 implementation with numerical atomic orbital basis functions: algorithm and benchmarks.* Submitted to Phys. Rev. Materials (Nov. 10, 2020).
602. *Regler, B., M. Scheffler, and L.M. Ghiringhelli: TCMI: a non-parametric mutual-dependence estimator for multivariate continuous distributions.* Submitted to Data Mining and Knowledge Discovery (Jan 30, 2020).
603. *Sutton, C., M. Boley, L. M. Ghiringhelli, M. Rupp, J. Vreeken, M. Scheffler: Identifying Domains of Applicability of Machine Learning Models within Materials Spaces.* Accepted on Nature Comm. (2020).
604. *Zacharias, M., M. Scheffler, and C. Carbogno: Fully Anharmonic, Non-Perturbative Theory of Vibronically Renormalized Electronic Band Structures.* Phys. Rev. B **102**, 045126 (2020).