# Bibliography

[1] S. Studer, S. Stucki, and J. D. Speight. Hydrogen as a fuel. In A. Züttel, A. Borgschulte, and L. Schlapbach, editors, *Hydrogen as a Future Energy Carrier*. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2008.

[2] A. Züttel. Hydrogen storage materials. *Naturwissenchaften*, 91:157–172, 2004.

[3] C. Read, G. Thomas, G. Ordaz, and S. Satyapal. U.S. Department of Energy's system targets for on-board vehicular hydrogen storage. *Material Matters*, 2(2):3–4, 2007. Material Matters is a publication of Aldrich Chemical Co., Inc.

[4] S. Satyapal, J. Petrovic, C. Read, G. Thomas, and G. Ordaz. The US Department of Energy's National Hydrogen Storage Project: Progress towards meeting hydrogen-powered vehicle requirements. *Catalysis Today*, 120(3-4):246–256, 2007.

[5] S. K. Bhatia and A. L. Myers. Optimum conditions for adsorptive storage. *Langmuir*, 22:1688, 2006.

[6] F. Rouquerol, J. Rouquerol, and K. Sing. *Adsorption by Powders and Porous Solids*. Academic Press, London, 1999.

[7] N. Stetson. (Private communication).

[8] J. K. Johnson and M. W. Cole. Hydrogen adsorption in single-walled carbon nanotubes. In E. J. Bottani and J. M. D. Tascón, editors, *Adsorption by Carbons*, chapter 15, pages 369–401. Elsevier, 2008.

[9] V. A. Parsegian. *Van der Waals Forces.* Cambridge University Press, New York, 2006.

[10] R. Lochan and M. Head-Gordon. Computational studies of molecular hydrogen binding affinities: The role of dispersion forces, electrostatics, and orbital interactions. *Phys. Chem. Chem. Phys.*, 8:1357–1370, 2006.

[11] G. J. Kubas. Fundamental of $H_2$ binding and reactivity on transition metals underlying hydrogenase function and $H_2$ production and storage. *Chem. Rev.*, 107:4152–4205, 2007.

[12] W. Zhou and T. Yildirim. Nature and tunability of enhanced hydrogen binding in metal-organic frameworks with exposed transition metal sites. *J. Phys. Chem. C Lett.*, 112:8132–8135, 2008.

[13] A. C. Dillon and M. J. Heben. Hydrogen storage using carbon adsorbents: past, present and future. *Appl. Phys. A*, 72:133, 2001.

[14] R. Ströbel, J. Garche, P. T. Moseley, L. Jörissen, and G. Wolf. Hydrogen storage by carbon materials. *J. Power Sources*, 159:781–801, 2006.

[15] E. L. Pace and A. R. Siebert. Heat of adsorption of parahydrogen and orthodeuterium on Graphon. *J. Phys. Chem.*, 63:1398–1400, 1959.

[16] Q. Wang and J. K. Johnson. Molecular simulation of hydrogen adsorption in single-walled carbon nanotubes and idealized carbon slit pores. *J. Chem. Phys.*, 110(1):577, 1999.

[17] M. Rzepka, P. Lamp, and M. A. de la Casa-Lillo. Physisorption of hydrogen on microporous carbon and carbon nanotubes. *J. Phys. Chem. B*, 102:10894–10898, 1998.

[18] S. Patchkovskii and T. Heine. Evaluation of the adsorption free energy of light guest molecules in nanoporous host strutures. *Phys. Chem. Chem. Phys.*, 9:2697–2705, 2007.

[19] M. G. Nijkamp, J. E. M. J. Raaymakers, A. J. van Dillen, and K. P. de Jong. Hydrogen storage using physisorption—materials demands. *Appl. Phys. A*, 72:619–623, 2001.

[20] B. Panella, M. Hirscher, and S. Roth. Hydrogen adsorption in different carbon nanostructures. *Carbon*, 43:2209–2214, 2005.

[21] F. S. Baker, C. E. Miller, A. J. Repik, and E. D. Tolles. Activated Carbon. In *Kirk-Othmer Encyclopedia of Chemical Technology*, volume 4, page 741. John Wiley and Sons, 2003.

[22] M. Felderhoff, C. Weidenthaler, R. von Helmolt, and U. Eberle. Hydrogen storage: The remaining scientific and technological challenges. *Phys. Chem. Chem. Phys.*, 9:2643–2653, 2007.

[23] S. H. Jhung, J. W. Yoon, J. S. Lee, and J.-S. Chang. Low-temperature adsorption/storage of hydrogen on FAU, MFI, and MOR zeolites with various Si/Al ratios: Effect of electrostatic field and pore structures. *Chem. Eur. J.*, 13(S):6502–6507, 2007.

[24] A. V. A. Kumar, H. Jobic, and S. Bhatia. Quantum effects of adsorption and diffusion of hydrogen and deuterium in microporous materials. *J. Phys. Chem. B*, 110:16666–16671, 2006.

[25] N. L. Rosi, J. Eckert, M. Eddaoudi, D. T. Vodak, J. Kim, M. O'Keeffe, and O. M. Yaghi. Hydrogen storage in microporous metal-organic frameworks. *Science*, 300:1127, 2003.

[26] H. K. Chae, D. Y. S.-P., J. Kim, Y. Go, M. Eddaoudi, A. J. Matzger, M. O'Keeffe, and O. M. Yaghi. A route to high surface area porosity and inclusion of large molecules in crystals. *Nature*, 427:523–527, 2004.

[27] H. Furukawa, M. A. Miller, and O. M. Yaghi. Independent verification of the saturation hydrogen uptake in MOF-177 and establishment of a benchmark for hydrogen adsorption in metal-organic frameworks. *J. Mater. Chem.*, 17:3197–3204, 2007.

[28] M. Dincă, A. Dailly, Y. Liu, C. M. Brown, D. A. Neumann, and J. R. Long. Hydrogen storage in a microporous metal-organic framework with exposed $Mn^{2+}$ coordination site. *J. Am. Chem. Soc.*, 126:16876–16883, 2006.

[29] Craig M. Brown, Yun Liu, Taner Yildirim, Vanessa K Peterson, and Cameron J Kepert. Hydrogen adsorption in HKUST-1: a combined inelastic neutron scattering and first-principles study. *Nanotechnology*, 20:204025, 2009.

[30] Y. Liu, H. Kabbour, C. M. Brown, D. A. Neumann, and C. C. Ahn. Increasing the density of adsorbed hydrogen with coordinatively unsaturated metal center in metal-organic frameworks. *Langmuir*, 24:4772–4777, 2008.

[31] A. Züttel, P. Sudan, P. Mauron, and P. Wenger. Model for the hydrogen adsorption on carbon nanostructures. *Appl. Phys. A*, 78:941–946, 2004.

[32] N. Texier-Mandoki, J. Dentzer, T. Piquero, S. Saadallah, P. David, and C. Vix-Guterl. Hydrogen storage in activated carbon materials: Role of the nanoporous texture. *Carbon*, 42:2744–2747, 2004.

[33] P. Bénard and R. Chahine. Storage of hydrogen by physisorption on carbon and nanostructured materials. *Scr. Mater.*, 56:803–808, 2007.

[34] A. Züttel, P. Sudan, Ph. Mauron, T. Kiyobayashi, Ch. Emmenegger, and L. Schlapbach. Hydrogen storage in carbon nanostructures. *Int. J. Hydrogen Energy*, 27(2):203–212, 2002.

[35] E. Poirier, R. Chahine, and T. K. Bose. Hydrogen adsorption in carbon nanostructures. *Int. J. Hydrogen Energy*, 26:831–835, 2001.

[36] Y. Zhao, Y.-H. Kim, A. C. Dillon, M. J. Heben, and S. B. Zhang. Hydrogen storage in novel organometallic buckyballs. *Phys. Rev. Lett.*, 94(15):155504, Apr 2005.

[37] T. Yildirim, J. Íñiguez, and S. Ciraci. Molecular and dissociative adsorption of multiple hydrogen molecules on transition metal decorated $C_{60}$. *Phys. Rev. B*, 72(15):153403, Oct 2005.

[38] I. Cabria, M. J. López, and J. A. Alonso. Hydrogen storage in pure and Li-doped carbon nanopores: Combined effects of concavity and doping. *J. Chem. Phys.*, 128(14):144704, 2008.

[39] W.-Q. Deng, X. Xu, and W. A. Goddard. New alkali doped pillared carbon materials designed to achieve practical reversible hydrogen storage for transportation. *Phys. Rev. Lett.*, 92(16):166103, 2004.

[40] Y. Zhao, Y.-H. Kim, L. J. Simpson, A. C. Dillon, S.-H. Wei, and M. J. Heben. Opening space for $H_2$ storage: Cointercalation of graphite with lithium and small organic molecules. *Phys. Rev. B*, 78(14):144102, 2008.

[41] S. Challet, P. Azaïs, R. J. M. Pellenq, O. Isnard, J. L. Soubeyroux, and L. Duclaux. Hydrogen adsorption in microporous alkali-doped carbons (activated carbon and single wall nanotubes). *J. Phys. Chem. Solids*, 65(2-3):541–544, 2004.

[42] F. E. Pinkerton, B. G. Wicke, C. H. Olk, G. G. Tibbetts, G. P. Meisner, M. S. Meyer, and J. F. Herbst. Thermogravimetric measurment of hydrogen adsorption in alkali-modified carbon materials. *J. Phys. Chem. B*, 104:9460–9467, 2000.

[43] K. Fredenhagen and G. Cadenbach. Die Bindung von Kalium durch Kohlenstoff. *Z. anorg. Chem.*, 158(1):249–263, 1926.

[44] A. Herold. Recherches sur les composes dinsertion du graphite. *Bull. Soc. Chim. Fr*, 187:999–1004, 1955.

[45] W. Rüdorff and E. Schulze. Über Alkaligraphitverbindungen. *Z. anorg. Chem.*, 277(3–4):156–171, 1954.

[46] D. E. Nixon and G. S. Parry. Formation and structure of the potassium graphites. *Brit. J. Appl. Phys. (J. Phys. D.)*, 1:291–299, 1968.

[47] A. Herold and D. Saehr. Effects of hydrogen on insertion compounds of graphite with alkali metals. *Compt. rend.*, 250:545, 1960.

[48] K. Watanabe, T. Kondow, M. Soma, T. Onishi, and K. Tamaru. Molecular-sieve type sorption on alkali graphite intercalation compounds. *Proc. R. Soc. London, Ser. A*, 333:51–67, 1973.

[49] P. Lagrange, D. Guerard, J. F. Mareche, and A. Herold. Hydrogen storage and isostopic protium-deuterium exchange in graphite-potassium intercalation compounds. *Journal of the Less-Common Metals*, 131:371–378, 1987.

[50] T. Terai and Y. Takahashi. Formulation of isotherms for low-temperature absorption of $H_2$ and $D_2$ on $KC_{24}$ prepared from natural graphite. *Synth. Met.*, 34:329–334, 1989.

[51] J. P. Beaufils, T. Crowley, T. Rayment, R. K. Thomas, and J. W. White. Tunnelling of hydrogen in alkali metal intercalation compounds. *Molecular Physics*, 44(6):1257–1269, 1981.

[52] L. Pauling. The rotational motion of molecules in crystals. *Physical Review*, 36(3):430–443, 1930.

[53] T. E. Stern. The symmetric spherical oscillator, and the rotational motion of homopolar molecules in crystals. *Proc. R. Soc. London, Ser. A*, 130(815):551–557, 1931.

[54] S. A. Solin and H. Zabel. The physics of ternary graphite intercalation compounds. *Advances in Physics*, 37(2):87–254, 1988.

[55] T. Enoki, S. Miyajima, M. Sano, and H. Inokuchi. Hydrogen-alkali-metal-graphite ternary intercalation compounds. *J. Mater. Res.*, 5(2):435–466, 1990.

[56] R. Nishitani, Y. Uno, and H. Suematsu. In situ observation of staging in potassium-graphite intercalation compounds. *Phys. Rev. B*, 27:6572, 1983.

[57] S. B. DiCenzo. Relaxed incommensurate structure of the intercalant layer in higher-stage graphite intercalation compounds. *Phys. Rev. B*, 26(10):5878–5881, 1982.

[58] Y. Arai, Y. Shirikawa, and S. Tamaki. Structural properties of low dimensional potassium metal in intercalated graphite. *Journal of Non-Crystalline Solids*, 205-207:803–806, 1996.

[59] J. B Hastings, W. D. Ellenson, and J. E. Fischer. Phase transitions in potassium-intercalated graphite: $KC_{24}$. *Physical Review Letters*, 42(23):1552, 1979.

[60] D. E. Nixon and G. S. Parry. Order-disorder transformation in potassium graphite. *Nature*, 216:909–910, 1967.

[61] F. Rousseaux, R. Moret, D. Guerard, and P. Lagrange. X-ray study of the liquid and solid phases of the alkali metals in $KC_{24}$ and $CsC_{24}$-intercalated graphite single crystals. *Phys. Rev. B*, 42(1):725, 1990.

[62] R. Clarke, J. N. Gray, H. Homma, and M. J. Winokur. Evidence for discommensurations in graphite intercalation compounds. *Phys. Rev. Lett.*, 47(19):1407, 1981.

[63] G. R. S. Naylor and J. W. White. Structure of second-stage graphite-rubidium, $C_{24}Rb$. *J. Chem. Soc., Faraday Trans.*, 83:3447–3458, 1987.

[64] A. Lovell, F. Fernandez-Alonso, N. T. Skipper, K. Refson, S. M. Bennington, and S. F. Parker. Quantum delocalization of molecular hydrogen in alkali-graphite intercalates. *Phys. Rev. Lett.*, 101:126101, 2008.

[65] A. P. Smith, R. Benedek, F. R. Trouw, and L. H. Yang M. Minkoff. Quasi-two-dimensional quantum states of $H_2$ in stage-2 Rb-intercalated graphite. *Phys. Rev. B*, 53(15):10187, 1996.

[66] J. J. Murray and A. R. Ubbelohde. Electronic properties of some synthetic metals derived from graphite. *Proc. Roy. Soc. A.*, 312:371–380, 1969.

[67] M. S. Dresselhaus and G. Dresselhaus. Intercalation compounds of graphite. *Advances In Physics*, 51(1):1–186, 2002.

[68] T. Terai and Y. Takahashi. Sorption of hydrogen isotopes on potassium-carbon intercalation compounds at low temperatures. *Synthetic metals*, 7:46–55, 1983.

[69] I. Cabria, M. J. López, and J. A. Alonso. Enhancement of hydrogen physisorption on graphene and carbon nanotubes by Li doping. *J. Chem. Phys.*, 123:204721, 2005.

[70] K. Ichimura, E. Takamura, and M. Sano. Hydrogen in alkali-metal-graphite intercalation compounds. *Synth. Met.*, 40:355–368, 1991.

[71] C. C. Ahn, J. J. Vajo, B. Fultz, R. Yazami, and D. W. Brown. Neutron diffraction of stage 2 and stage 4 deuterided K-intercalated graphite at Los Alamos National Laboratory. Technical report, LANSCE Proposal # 20011042, 2002.

[72] A. J. Kidnay and M. J. Hiza. High pressure adsorption isotherms of neon, hydrogen, and helium at 76 K. *Adv. Cryog. Eng.*, 12:730–740, 1967.

[73] L. Zhou. Adsorption isotherms for the supercritical region. In József Tóth, editor, *Adsorption: Theory, Modeling, and Analysis*, volume 107 of *Surfactant Science Series*, page 211. Marcel Dekker, Inc., 2002.

[74] L. Czepirski and J. Jagiello. Virial-type thermal equation of gas-solid adsorption. *Chem. Eng. Sci.*, 44:797–801, 1989.

[75] H. W. Brinks, A. Fossdal, R. C. Bowman, and B. C. Hauback. Pressure–composition isotherms of $TbNiAlH_x$. *J. Alloys Compd.*, 417(1-2):92–95, 2006.

[76] E. W. Lemmon, M. L Huber, and M. O. McLinden. *NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties-REFPROP*. Number Version 8.0 in Standard Reference Data Program. National Institute of Standards and Technology, Gaithersburg, 2007.

[77] T. P. Blach and E. M. Gray. Sieverts apparatus and methodology for accurate determination of hydrogen uptake by light-atom hosts. *J. Alloys Compd.*, 446-447:692–697, 2007.

[78] B. Fultz and J. M. Howe. *Transmission Electron Microscopy and Diffractometry of Materials*. Springer, 2002.

[79] G. L. Squires. *Introduction to the Theory of Thermal Neutron Scattering*. Cambridge University Press, 1978.

[80] J. R. D. Copley, D. A. Neumann, and W. A. Kamitakahara. Energy distributions of neutrons scattered from $C_{60}$ using the beryllium detector method. *Can. J. Phys.*, 73:763, 1995.

[81] J. R. D. Copley and J. C. Cook. The disk chopper spectrometer at NIST: a new instrument for quasielastic neutron scattering studies. *Chem. Phys.*, 292:477, 2003.

[82] W. Zhou, H. Wu, M. R. Hartman, and T. Yildirim. Hydrogen and methane adsorption in metal-organic frameworks: A high-pressure volumetric study. *J. Phys. Chem. C*, 111(44):16131–16137, 2007.

[83] G. H. Vineyard. Scattering of slow neutrons by a liquid. *Phys. Rev.*, 110:999–1010, 1958.

[84] R. Stockmeyer, H. J. Stortnik, and H. M. Conrad. Diffusive motions of molecules on catalytic surfaces. In *Proceedings of conference on neutron scattering*, page 303, Gatlinburg, Tennessee, 1976.

[85] P. L. Hall and D. K. Ross. Incoherent neutron scattering function for molecular diffusion in lamellar systems. *Mol. Phys.*, 36(5):1549–1554, 1978.

[86] C. T. Chudley and R. J. Elliott. Neutron scattering from a liquid on a jump diffusion model. *Proc. Phys. Soc. London*, 77:353, 1961.

[87] J. M. Rowe, K. Sköld, and H. E. Flotow. Quasielastic neutron scattering by hydrogen in the $\alpha$ and $\beta$ phase of vanadium hydride. *J. Phys. Chem. Solids*, 32:41–54, 1971.

[88] D. K. Ross. Neutron scattering studies of metal-hydrogen systems. In H. Wipf, editor, *Topics in Applied Physics, Vol. 73*, page 153. Springer-Verlag, Berlin, Heidelberg, 1997.

[89] U. Stuhr, H. Wipf, R. K. Kremer, H. Mattausch, A. Simon, and J. C. Cook. A neutron-spectroscopy study of two-dimensional hydrogen diffusion in the hydride halide $YBrH_{0.78}$. *J. Phys.: Condens. Matter*, 6:147–158, 1994.

[90] R. E. Lechner. Effects of low-dimensionality in solid-state protonics conductors. *Solid State Ionics*, 77:280–286, 1995.

[91] A. J. Dianoux and F. Volino. Incoherent scattering law for neutron quasi-elastic scattering in liquid crystals. *Mol. Phys.*, 30(4):1181–1194, 1975.

[92] A. Meyer, R. M. Dimeo, P. M. Gehring, and D. A. Neumann. The High Flux Backscattering Spectrometer at the NIST Center for Neutron Research. *Rev. Sci. Instrum.*, 74:2759, 2003.

[93] J. D. Gale and A. L. Rohl. The general utility lattice program. *Mol. Simul.*, 29:291, 2003.

[94] G. Chen, Y. Guo, N. Karasawa, and W. A. Goddard III. Electron-phonon interactions and superconductivity in $K_3C_{60}$. *Phys. Rev. B*, 48:13959–13970, 1993.

[95] T. Róg, K. Murzyn, K. Hinsen, and G. R. Kneller. nMoldyn: A program package for a neutron scattering oriented analysis of molecular dynamics simulations. *Journal of computational chemistry*, 24(5):657–667, 2003.

[96] D. G. Narehood, J. V. Pearce, P. C. Eklund, P. E. Sokol, R. E. Lechner, J. Pieper, J. R. D. Copley, and J. C. Cook. Diffusion of $H_2$ adsorbed on single-walled carbon nanotubes. *Phys. Rev. B*, 67:205409, 2003.

[97] O.-E. Haas, J. M. Simon, S. Kjelstrup, A. L. Ramstad, and P. Fouquet. Quasielastic neutron scattering investigation of the hydrogen surface self-diffusion on polymer electrolyte membrane fuel cell catalyst support. *J. Phys. Chem. C*, 112:3121–3125, 2008.

[98] R. Kahn and E. Viennet E. C. De Lara. Diffusivity of the hydrogen molecule sorbed in NaA Zeolite by a neutron scattering experiment. *J. Chem. Phys.*, 91(8):5097–5102, 1989.

[99] H. Fu, F. Trouw, and P. E. Sokol. A quasi-elastic and inelastic neutron scattering study of $H_2$ in zeolite. *J. Low Temp. Phys.*, 116(3/4):149–165, 1999.

[100] F. Salles, H. Jobic, G. Maurin, MM Koza, PL Llewellyn, T. Devic, C. Serre, and G. Ferey. Experimental evidence supported by simulations of a very high $H_2$ diffusion in metal organic framework materials. *Physical Review Letters*, 100(24):245901, 2008.

[101] A. V. Skripov, M. A. Gonzalez, and R. Hempelmann. Evidence for a two-site localized hydrogen motion in C15-type $YMn_2H_2$. *J. Phys.: Condens. Matter*, 18:7249–7256, 2006.

[102] F. Fernandez-Alonso, F. J. Bermejo, C. Cabrillo, R. O. Loutfy, V. Leon, and M. L. Saboungi. Nature of the bound states of molecular hydrogen in carbon nanohorns. *Phys. Rev. Lett.*, 98:215503, 2007.

[103] H. Freimuth, H. Wichert, and H. J. Lauter. The commensurate-incommensurate transition of hydrogen monolayers physisorbed on graphite. *Surface Science*, 189/190:548–556, 1987.

[104] S. N. Coppersmith, D. S. Fisher, B. I. Halperin, P. A. Lee, and W. F. Brinkman. Dislocations and the commensurate-incommensurate transition in two dimensions. *Phys. Rev. B*, 25(1):349–363, 1982.

[105] J. M. Kosterlitz and D. J. Thouless. Ordering, metastability and phase transitions in two-dimensional systems. *J. Phys. C: Solid State Phys.*, 6:1181–1203, 1973.

[106] B. I. Halperin and D. R. Nelson. Theory of two-dimensional melting. *Phys. Rev. Lett.*, 41(2):121–124, 1978.

[107] K.J. Strandburg. Two-dimensional melting. *Rev. Mod. Phys.*, 60(1):161–207, 1988.

[108] H. Zabel, A. Magerl, J. J. Rush, and M. E. Misenheimer. Diffusion and melting in two dimensions: A quasielastic neutron scattering study of alkali metals in graphite. *Phys. Rev. B*, 40(11):7616–7632, 1989.

[109] Y. J. Glanville, J. V. Pearce, P. E. Sokol, B. Newalker, and S. Komarneni. Study of $H_2$ confined in the highly ordered pores of MCM-48. *Chem. Phys.*, 292:289–293, 2003.

[110] C. Cohen-Tannoudji, B. Diu, and F. Laloë. *Quantum Mechanics*, volume 1, chapter 6, pages 712–726. Wiley-Interscience, 1977.

[111] J. A. Young and J. U. Koppel. Show neutron scattering by molecular hydrogen and deuterium. *Phys. Rev.*, 135(3A):603–611, 1964.

[112] I. P. Jackson and J. W. White. Domain mobility and rotational tunneling of hydrogen in graphite intercalates. *Chem. Phys. Lett.*, 1987:397–399, 134.

[113] G. Kresse and J. Furthmüller. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. *Phys. Rev. B*, 54(16):11169–11186, Oct 1996.

[114] J. P. Perdew, K. Burke, and M. Ernzerhof. Generalized gradient approximation made simple. *Phys. Rev. Lett.*, 77(18):3865–3868, Oct 1996.

[115] C. C. Marston and G. G. Balint-Kurti. The Fourier grid Hamiltonian method for bound state eigenvalues and eigenfunctions. *J. Chem. Phys.*, 91:3571, 1989.

[116] P. C. H. Mitchell, S. F. Parker, A. J. Ramirez-Cuesta, and J. Tomkinson. *Vibrational Spectroscopy with Neutrons*, chapter 6. World Scientific, Singapore, 2005.

[117] W. J. Stead, I. P. Jackson, J. McCaffrey, and J. W. White. Tunnelling of hydrogen in alkali-metal-graphite intercalation compounds. *J. Chem. Soc., Faraday Trans. 2*, 84(10):16669–1682, 1988.

[118] C.J. Carlile, G.J. Kearley, G. Lindsell, and J.W. White. Structural and dynamics aspects of the tunnelling of hydrogen in caesium-intercalated graphite. *Physica B*, 241-243:491–494, 1998.

[119] S. Grimme. Semiempirical GGA-type density functional constructed with a long-range dispersion correction. *Journal of computational chemistry*, 27(15):1787, 2006.

[120] `http://charm.cs.uiuc.edu/OpenAtom/`.

[121] H. S. Cheng, A. C. Cooper, G. P. Pez, M. K. Kostov, P. Piotrowski, and S. J. Stuart. Molecular dynamics simulations on the effects of diameter and chirality on hydrogen adsorption in single-walled carbon nanotubes. *J. Phys. Chem. B*, 109:3780, 2005.

[122] A. Gigras, S. K. Bhatia, A. V. Anil Kumar, and A. L. Myers. Feasibility of tailoring for high isosteric heat to improve effectiveness of hydrogen storage in carbons. *Carbon*, 45:1043, 2007.

[123] F. Stoeckli, T. A. Centeno, A. B. Fuertes, and J. Muniz. Porous structure of polyarylamide-based activated carbon fibers. *Carbon*, 34:1201, 1996.

[124] M. A. Daley, D. Tandon, J. Economy, and E. J. Hippo. Elucidating the porous structure of activated carbon fibers using direct and indirect methods. *Carbon*, 34(10):1191–1200, 1996.

[125] J. I. Paredes, A. Martínez-Alonso, and J. M. D. Tascón. Characterization of microporosity and mesoporosity in carbonaceous materials by scanning tunneling microscopy. *Langmuir*, 17:474, 2001.

[126] R. T. Yang. *Adsorbents: Fundamental and Applications*. Wiley Interscience, Hoboken, New Jersey, 2003.

[127] J. P. Olivier. Improving the models used for calculating the size distribution of micropore volume of activated carbons from adsorption data. *Carbon*, 36:1469, 1998.

[128] H. Kabbour, T. F. Baumann, J. H. Satcher Jr., A. Saulnier, and C. C. Ahn. Toward new candidates for hydrogen storage: High-surface-area carbon aerogels. *Chem. Mater.*, 18(26):6085, 2006.

[129] T. X. Nguyen and S. K. Bhatia. Characterization of activated carbon fibers using argon adsorption. *Carbon*, 43:775, 2005.

[130] A. Züttel, A. Borgschulte, and S.I. Orimo. Tetrahydroborates as new hydrogen storage materials. *Scr. Mater.*, 56(10):823–828, 2007.

[131] J. J. Vajo, S. L. Skeith, and F. Mertens. Reversible storage of hydrogen in destabilized $LiBH_4$. *J. Phys. Chem. B*, 109(9):3719–3722, 2005.

[132] J. J. Vajo, F. Mertens, C. C. Ahn, R. C. Bowman, and B. Fultz. Altering hydrogen storage properties by hydride destabilization through alloy formation: LiH and $MgH_2$ destabilized with Si. *J. Phys. Chem. B*, 108(37):13977–13983, 2004.

[133] J. J. Vajo and G. L. Olson. Hydrogen storage in destabilized chemical systems. *Scr. Mater.*, 56(10):829–834, 2007.

[134] J. J. Vajo, T. T. Salguero, A. F. Gross, S. L. Skeith, and G. L. Olson. Thermodynamic destabilization and reaction kinetics in light metal hydride systems. *J. Alloys Compd.*, 446:409–414, 2007.

[135] F. Pinkerton, M. Meyer, G. Meisner, M. Balogh, and J. Vajo. Phase boundaries and reversibility of $LiBH_4/MgH_2$ hydrogen storage material. *J. Phys. Chem. C*, 111(35):12881–12885, 2007.

[136] J. Yang, A. Sudik, and C. Wolverton. Destabilizing $LiBH_4$ with a Metal (M= Mg, Al, Ti, V, Cr, or Sc) or Metal Hydride ($MH_2$= $MgH_2$, $TiH_2$, or $CaH_2$). *J. Phys. Chem. C*, 111(51):19134–19140, 2007.

[137] S. V. Alapati, J. K. Johnson, and D. S. Sholl. Stability analysis of doped materials for reversible hydrogen storage in destabilized metal hydrides. *Phys. Rev. B*, 76(10):104108, 2007.

[138] S. V. Alapati, J. K. Johnson, and D. S. Sholl. Using first principles calculations to identify new destabilized metal hydride reactions for reversible hydrogen storage. *Phys. Chem. Chem. Phys.*, 9(12):1438–1452, 2007.

[139] D. J. Siegel, C. Wolverton, and V. Ozoliņš. Thermodynamic guidelines for the prediction of hydrogen storage reactions and their application to destabilized hydride mixtures. *Phys. Rev. B*, 76(13):134102, 2007.

[140] S. V. Alapati, J. K. Johnson, and D. S. Sholl. First principles screening of destabilized metal hydrides for high capacity $H_2$ storage using scandium. *J. Alloys Compd.*, 446:23–27, 2007.

[141] A. E. Bennett, C. M. Rienstra, M. Auger, K. V. Lakshmi, and R. G. Griffin. Heteronuclear decoupling in rotating solids. *J. Chem. Phys.*, 103(16):6951–6958, 1995.

[142] A. Züttel, P. Wenger, S. Rentsch, P. Sudan, P. Mauron, and C. Emmenegger. $LiBH_4$: a new hydrogen storage material. *J. Power Sources*, 118(1-2):1–7, 2003.

[143] S. Orimo, Y. Nakamori, N. Ohba, K. Miwa, M. Aoki, S. Towata, and A. Züttel. Experimental studies on intermediate compound of $LiBH_4$. *Appl. Phys. Lett.*, 89(2):021920, 2006.

[144] S. J. Hwang, R. C. Bowman Jr, J. W. Reiter, J. Rijssenbeek, G. L. Soloveichik, J. C. Zhao, H. Kabbour, and C. C. Ahn. NMR Confirmation for formation of $[B_{12}H_{12}]^{2-}$ complexes during hydrogen desorption from metal borohydrides. *J. Phys. Chem. C*, 112:3164–3169, 2008.

[145] N. Ohba, K. Miwa, M. Aoki, T. Noritake, S. Towata, Y. Nakamori, S. Orimo, and A. Züttel. First-principles study on the stability of intermediate compounds of $LiBH_4$. *Phys. Rev. B*, 74(7):075110, 2006.

[146] M. Dornheim, S. Doppiu, G. Barkhordarian, U. Boesenberg, T. Klassen, O. Gutfleisch, and R. Bormann. Hydrogen storage in magnesium-based hydrides and hydride composites. *Scr. Mater.*, 56(10):841–846, 2007.

[147] U. Bösenberg, S. Doppiu, L. Mosegaard, G. Barkhordarian, N. Eigen, A. Borgschulte, T.R. Jensen, Y. Cerenius, O.Gutfleisch, T. Klassen, M. Dornheim, and R. Bormann. Hydrogen sorption properties of $MgH_2$-$LiBH_4$ composites. *Acta Mater.*, 55(11):3951–3958, 2007.

[148] C. Kempter and J. McGuire. U.S. Patent 3,152,868. Preparation of Scandium Hydrides, 1964.

[149] Estimate of equilibrium compositions made using *Outokumpu HSC Chemistry* for Windows, version 4.0 (ChemSC, Inc., 1999).

[150] V. Bérubé, G. Radtke, M. Dresselhaus, and G. Chen. Size effects on the hydrogen storage properties of nanostructured metal hydrides: A review. *Int. J. Energy Res.*, 31(6):637–663, 2007.