

**Harold H. Schobert**  
**www.thecoalguy.com**

**Present positions:**

- Chief Scientist, Schobert International LLC, State College, PA (since 2006)
- Extraordinary Professor, Coal and Laser Chemistry Group, School of Physical and Chemical Sciences, North-West University, Potchefstroom, South Africa (since 2006)

**Management and organizational experience:**

Director, The Energy Institute, Penn State University (1998–2006). Held ultimate responsibility for directing the activities of a research unit with a staff of 130 faculty, international visiting scientists, research staff, support staff, and students. Annual budget was \$10–12 million in external funding, representing a 20:1 leveraging of state-appropriated funds. This was a tripling of the budget that had existed under the previous director. Principal research activities of the Institute included coal-to-liquids, catalysis, fuel cells, stationary combustion, internal combustion engines, biomass energy, petroleum and natural gas engineering, and carbon materials. The Institute established three parallel federal:industrial:academic research consortia that eventually involved over a hundred companies. Also established working relationships with industrial organizations, such as the Pennsylvania Coal Association and Pennsylvania Oil and Gas Association. Provided briefings and hosted visits for state and federal legislators on various energy issues.

Chair, Fuel Science Program, Department of Materials Science and Engineering, Penn State University (1988–1996). Held overall responsibility for oversight of this academic program, involving eight active tenured or tenure-track faculty, plus clerical and technician support. The faculty were responsible for undergraduate and graduate education in fuel science, including, e.g., combustion science and engineering, fuel chemistry and technology, and carbon materials, as well as introductory course in energy for non-scientists. Established a novel energy and fuels engineering “option” with Chemical Engineering, developing a curriculum that combined the core principles of chemical engineering with fuel science. Established a student exchange program with Nottingham-Trent University (UK).

Manager, Coal Science Division, Energy Research Center, University of North Dakota (1983–1986). Held overall responsibility for managing this group, which was newly created in 1983. Built the group up to include approximately 25 scientists and engineers at Ph.D., M.S. or B.S. level. Research activities were studies of geochemistry, organic chemistry, solvent extraction, pyrolysis, physical properties, and formation and behavior of ashes and slags from lignites and subbituminous coals. Within three years this group was publishing more papers per year than the Chemical Engineering department, and outpaced all other divisions of the Energy Research Center in dollar value of proposals submitted, by a factor of four.

Manager, Analytical Research Division, Grand Forks Energy Technology Center, US DOE (1978–1983). Held overall responsibility for managing this group of 20–25 scientists at Ph.D., M.S. or B.S. level. Managed the transition of this division from a classical “wet chemistry” analytical group in 1978 to a unit fully equipped with (then) state-of-the-art instrumentation for organic, inorganic, and surface analyses relevant to low-rank coal technology. The division took on self-generated research projects in development of new analytical methods for characterization of low-rank coals and their reaction products. The division also had responsibility for analytical support to GFETC’s technology projects in gasification, direct liquefaction, pulverized-coal and fluidized-bed combustion, SO<sub>x</sub> scrubbing, and ash collection.

**Other professional experience (without management responsibilities):**

Chief Scientist, Schobert International LLC (2006-present). Provide consulting services on coal research and development, including providing expert witness services and testimony, critical reviews of the literature, and working with clients on designing experimental and test plans for various coal conversion processes.

Associate Professor, Professor, Professor Emeritus of Fuel Science, Penn State University, University Park, PA (1986-2011). Responsible for teaching undergraduate and graduate courses in chemistry of fuels, energy conversion processes, coal structure, and energy for non-science students. Responsible for overseeing undergraduate and research projects leading to honors undergraduate theses, or M.S. and Ph.D. theses.

Research Chemist, Grand Forks Energy Research Center, US DOE/ERDA (1976–1978). Responsible for conducting hands-on research projects relevant to coal gasification, including environmental effects, pilot plant operation, refractory corrosion, and slaw flow behavior.

Research Chemist, Deepsea Ventures Inc., Gloucester Point, VA (1972–1976). Responsible for conducting hands-on research projects in pyro- and hydrometallurgy, with particular respect to manganese, molybdenum, and vanadium. Projects included design, construction, and operation of pilot plants.

Instructor, Department of Chemistry, Iowa State University (1970–1972). Responsible for lecturing and laboratory supervision in general chemistry. Involved in creating one of the nation's first systems for closed-circuit televised lectures in laboratory practice.

**Education:**

Ph.D., Inorganic Chemistry, Iowa State University (1965–1970). Thesis research was on synthesis and characterization of novel thiolate complexes of osmium. Adviser: Prof. Robert E. McCarley.

B.S. Chemistry, Bucknell University (1961–1965).

**Significant state, national, and international boards and collaborations:**

Study on Alternative Liquid Fuels, National Petroleum Council (2010-2011). This study was commissioned by Secretary of Energy Chu, for evaluation for future liquid fuel potential. Served as a subject matter expert on coal-to-liquids technologies.

Panel on Alternative Liquid Transportation Fuels, National Research Council (2007-2009). Served on this panel, which was a subset of the major NAS/NAE study on America's Energy Future. Panel discussed and reviewed production of liquid fuels from fossil and biomass resources, and fossil/biomass coprocessing, including supply constraints and environmental issues. This panel's report emerged from the NRC review process in March '09.

Organizing Committee, 2009 International Conference on Coal Science and Technology (2007-2009). The only American scientist selected for membership on this board. The board was involved in all aspects of this conference, including technical programming, site selection (Cape Town, South Africa), manuscript review, and operation of the conference.

International Advisory Board, Synfuels and Coal Technology, Sasol R&D, Sasolburg, South Africa (2005–2008). The only American scientist selected for membership on this board. The board

provided review of on-going research programs and advice on research directions on matters impacting raw gas production from coal for the world's largest synthetic fuel company.

Extraordinary Professor of Natural Sciences, North-West University, Potchefstroom, South Africa (2006-present). Principal duties include co-advising of Ph.D., M.S. and fourth-year B.S. honors students in various aspects of coal chemistry; presenting ad hoc lectures or participating in short courses on coal science and technology; interacting with NWU faculty to build up teaching and research capacity in coal; and interacting with South African mining, electricity generation, and synthetic fuels companies to develop research programs.

Visiting Professor, Department of Chemistry, Çukurova University, Adana, Turkey (2002). Principal responsibilities were one-on-one interactions with graduate students in fuel chemistry, as well as presenting formal lectures on aspects of coal-to-liquids technology. Recruited two graduate students to Penn State as postdoctoral scholars.

Joint State Government Energy Strategy Working Group, Commonwealth of Pennsylvania (2001-2002). This group discussed and reviewed all aspects of energy use in Pennsylvania, including fossil fuels, biomass, hydropower, wind, and solar energy. Recommended strategies to insulate the state against major energy upheavals such as an oil embargo. Several recommendations of the group were eventually enacted into various state legislation.

Visiting Professor, Department of Applied Chemistry, Osaka University, Osaka, Japan (1993). Principal responsibilities included presentation of two short courses, one on coal chemistry and one on writing scientific papers in English; one-on-one interactions with graduate students in coal chemistry and applied organic chemistry; lecturing on coal chemistry at other universities and national laboratories in Japan.

Visiting Lecturer, NATO Advanced Summer School, Akçay, Turkey (1993). Presented lectures to this summer school on various aspects of coal chemistry and catalysis.

Deputy Chair, International Advisory Board, Institute of Coal Chemistry, Kemorovo, Siberia, Russia (1991–1993). The only American coal scientist selected for service on this board. Principal activities of the board were to provide technical advice on the establishment of a reference collection and sample bank of Russian coals, internationally accepted methods of characterizing coals, and impacts on Russian coal export markets. Served as deputy to the in-country chairman.

Energy Engineering Board, National Research Council (1990–1996). Among many other activities, participated in NRC reviews of DOE programs in energy efficiency and renewables, and in coal research.

### **Major research involvement:**

Development of coal-based jet fuel. Directed and coordinated a 20-year, \$40-million project that successfully developed a coal-based replacement for Jet A and JP-8 fuels. The project was taken from a preliminary white paper to pilot-plant production of prototype fuels to successful tests in a commercial aviation gas turbine engine. Byproducts include clean, low-sulfur diesel fuel. Work involved coordination of up to 30 people per year, including five to seven faculty members and up to four active subcontracts. The project was completed *at one-third under budget*. The project also resulted in publication of nearly 100 peer-reviewed papers by various faculty members, and well over a hundred publications in conference proceedings or presentations at professional meetings. Educational opportunities were provided for several dozen graduate students to receive M.S. or Ph.D. degrees, as well as specialized training for postdoctoral researchers. Former graduate students supported on this project are now employed at, e.g. BP, Chevron, ConocoPhillips, Ford, Naval Research Laboratory, and Pacific Northwest National Laboratory.

### **Awards and personal achievements:**

2010. Fellow, American Chemical Society. Elected by vote of the society to the second-ever class of Fellows; nominated by the Division of Fuel Chemistry.

2009. Distinguished Service Award, Division of Fuel Chemistry, American Chemical Society. Awarded for lifetime excellence in service to the division, including seven elective or appointive offices and contribution of over one hundred papers to the division's preprints for national ACS meetings.

2004. Henry H. Storch Award, Division of Fuel Chemistry, American Chemical Society. Awarded for lifetime excellence in fuel chemistry. This award is generally considered the most prestigious award in fuel science.

2004. Fred Cannon/Sloan Foundation Award for Commitment to Opportunities for Minority Students in Graduate Education. Awarded for building up enrollment and research opportunities for student from under-represented groups in energy and fuels education.

2002. Matthew and Anne Wilson Award for Excellence in Research, College of Earth and Mineral Sciences, Penn State University. Awarded for leadership of, and contributions to, the coal-based jet fuel program.

2001. Election to Phi Kappa Phi Honorary Society. Election for commitment to excellence in engineering education and research.

1996. Golden Key Honor Society Award for Penn State's Outstanding Faculty Member. Awarded primarily for teaching of upper level courses in fuel chemistry.

1988. Richard A. Glenn Award for Best Paper in Fuel Chemistry, Division of Fuel Chemistry, American Chemical Society, 3<sup>rd</sup> North American Chemical Congress. Awarded for a paper on high-temperature physical chemistry of coal ash.

1988. Matthew and Anne Wilson Award for Excellence in Teaching, College of Earth and Mineral Sciences, Penn State University. Awarded primarily for teaching of upper level courses in fuel chemistry.

1982. Award for Sustained Superior Performance, US DOE. Awarded for transformation of GFETC analytical research division from classical wet chemistry to fully modernized and instrumented group.

### **Books published**

1. Hutton, W. and H.H. Schobert, *Experimental Chemistry*, Collegiate Publishing Inc., Columbus, OH, 366 pages, 1978. *A laboratory manual for general chemistry courses.*
2. Schobert, H.H., *The Chemistry of Low-Rank Coals*, American Chemical Society, Washington, 315 pages, 1984. *An edited collection of chapters from a symposium on this topic sponsored by American Chemical Society.*
3. Schobert, H.H., *Coal: The Energy Source of Past and Future*, American Chemical Society, Washington, 298 pp., 1987. *A book on all aspects of coal technology, for non-specialist readers with no science background.*

4. Schobert, H.H., *The Chemistry of Hydrocarbon Fuels*, Butterworth-Heinemann, London, 348 pp., 1990. *A textbook on applied organic and physical chemistry of fuels, for college seniors or beginning graduate students; also for interested professional readers.*
5. Radovic, L.R. and H.H. Schobert, *Energy and Fuels in Modern Society*, McGraw-Hill, New York, 442 pp., 1991. *A textbook intended for an introductory course in energy for first-year college students.*
6. Schobert, H.H., K.D. Bartle, and L.J. Lynch, *Coal Science II*, American Chemical Society, Washington, 337 pp., 1991. *An edited collection of chapters from a symposium on this topic sponsored by American Chemical Society.*
7. Schobert, H.H. *Lignites of North America*. Elsevier Science Publishers, Amsterdam, 1995, 714 pp. *A comprehensive monograph on all aspects of science, technology, and utilization of lignites.*
8. Schobert, H.H. *Energy and Society: An Introduction*. Taylor and Francis, New York, 2002, 656pp. *A textbook covering all aspects of energy—fossil, nuclear, biomass, and renewables—for students with no science background; also for the interested general reader.*
9. Schobert, H.H. *Chemistry of Fossil and Biofuels*. Cambridge University Press, Cambridge, 2013. *A thorough revision and updating of the hydrocarbon fuels book, with substantially expanded coverage of biofuels.*
10. Schobert, H.H.: *Energy: The Basics*. Routledge: London, 2014. *A brief introduction to the science of energy for non-scientists.*
11. Schobert, H.H. *Energy and Society, Second Edition*. Taylor and Francis, 2014. *A thorough revision of the first edition, with updated and revised chapters on global warming, other environmental issues, and renewable or alternative energy sources.*

**Peer-reviewed research publications, arranged by topic:**

*(Through summer 2015.)*

Activated carbon

1. Gergova, K., S. Eser, and H.H. Schobert. Preparation and characterization of activated carbons from anthracite. *Energy and Fuels*, vol. 7, pp. 661-668, 1993.
2. Gergova, K., S. Eser, H.H. Schobert, M. Klimkiewicz, and P.W. Brown. Environmental scanning electron microscopy of activated carbon production from anthracite by one-step pyrolysis-activation. *Fuel*, vol. 74, pp. 1042-1048, 1995.
3. Zhang, Y., Z. Lu, M.M. Maroto-Valer, J.M. Andrésen, and H.H. Schobert. Comparison of high-unburned-carbon fly ashes from different combustor types and their steam activated products. *Energy and Fuels*, vol. 17, pp. 369-377, 2003.
4. Lu, Z., M.M. Maroto-Valer, and H.H. Schobert. Role of active sites in the steam activation of high unburned carbon fly ashes. *Fuel*, vol. 87, pp. 2598-2605, 2008.

5. Lu, Z.; M.M. Maroto-Valer; and H.H. Schobert. Catalytic effects of inorganic compounds on the development of surface areas of fly ash carbon during steam activation. *Fuel*, vol. 89, pp. 3436-3441, 2010.

#### Carbon dioxide capture

1. Indraknati, V.P., J.D. Kubicki, and H.H. Schobert. Quantum chemical modeling of ground states of CO<sub>2</sub> chemisorbed on anatase (001), (101), and (010) TiO<sub>2</sub> surfaces. *Energy and Fuels*, vol. 22, pp. 2611-2618, 2008.
2. Van Essendelft, D.T. and H.H. Schobert. Kinetics of the acid digestion of serpentine with concurrent grinding. 1. Initial investigations. *Industrial and Engineering Chemistry*, vol. 48, pp. 2556-2565, 2009.
3. Indrakanti, V.P., J.D. Kubicki, and H.H. Schobert. Photoinduced activation of CO<sub>2</sub> on Ti-based heterogeneous catalysts: current state, chemical physics based insights, and activation. *Energy and Environmental Science*, vol. 2, pp. 745-758, 2009.
4. Van Essendelft, D.T. and H.H. Schobert. Kinetics of the acid digestion of serpentine with concurrent grinding. Part 2. Detailed investigation and model development. *Industrial and Engineering Chemistry*, vol. 48, pp. 9892-9901, 2009.
5. Indraknati, V.P., J.D. Kubicki, and H.H. Schobert. Quantum mechanical modeling of CO<sub>2</sub> interactions with irradiated stoichiometric and oxygen-deficient TiO<sub>2</sub> surfaces: implications for the photocatalytic reduction of CO<sub>2</sub>. *Energy and Fuels* vol. 23, pp. 5247-5256, 2009.
6. Van Essendelft, D.T. and H.H. Schobert. Kinetics of the acid digestion of serpentine with concurrent grinding. Part 3. Model validation and prediction. *Industrial and Engineering Chemistry*, vol. 49, pp. 1588-1590, 2010.
7. Indrakanti, V.P., J.D. Kubicki, and H.H. Schobert. Photoinduced activation of CO<sub>2</sub> on TiO<sub>2</sub> surfaces: Quantum chemical modeling of CO<sub>2</sub> adsorption on oxygen vacancies. *Fuel Processing Technology*, vol. 92, pp. 805-811, 2011.

#### Catalyst development

1. Garcia, A.B. and H.H. Schobert, Comparative performance of impregnated molybdenum-sulfur catalysts in hydrogenation of Spanish lignite, *Fuel*, vol. 68, pp. 1613-1616, 1989.
2. Hayward, N. and H.H. Schobert, Thia crown ether complexes as catalyst precursors for direct liquefaction. *Energy and Fuels*, vol. 7, pp. 326-327, 1993.
3. Artok, L., P.B. Malla, S. Komarneni, and H.H. Schobert, Intercalated metal-clay catalysts in direct liquefaction of bituminous coal, *Energy and Fuels*, vol. 7, pp. 430-431, 1993.
4. Song, C., D.S. Parfitt, and H.H. Schobert. Bimetallic dispersed sulfide catalysts from organometallic clusters for coal liquefaction. *Catalysis Letters*, vol. 21, pp. 27-34, 1993.
5. Song, C., D.S. Parfitt, and H.H. Schobert. Bimetallic dispersed catalysts from molecular precursors containing Mo-Co-S for coal liquefaction. *Energy and Fuels*, vol. 8, pp. 313-319, 1994.

6. Cooke, W.S., E. Schmidt, C. Song, and H.H. Schobert. Reactions of dibenzothiophene with hydrogen in the presence of selected molybdenum, iron, and cobalt compounds. *Energy and Fuels*, vol. 10, pp. 591-596, 1996.
7. Schmidt, E., C. Song, and H.H. Schobert. Hydrotreatment of 4-(1-naphthylmethyl)bi-benzyl in the presence of iron catalysts and sulfur. *Energy and Fuels*, vol. 10, pp. 597-602, 1996.
8. Dutta, R.P. and H. H. Schobert. Hydrogenation/dehydrogenation of polycyclic aromatic hydrocarbons using ammonium tetrathiomolybdate as catalyst precursor. *Catalysis Today*, vol. 31, pp. 65-77, 1996.
9. Kirby, S.R., C. Song, and H.H. Schobert. Hydrodeoxygenation of O-containing polycyclic model compounds using a novel organometallic catalyst precursor. *Catalysis Today*, vol. 31, pp. 121-135, 1996.
10. Song, C., X. Ma, A.D. Schmitz, and H. H. Schobert. Shape-selective isopropylation of naphthalene over mordenite catalysts. Computational analysis using MOPAC. *Applied Catalysis A: General*, vol. 182 (1), pp. 175-181, 1999.
11. Medina, F.A., J.W. Larsen, H.H. Schobert, and J. Stuart. Coals catalyze the reduction of nitroaromatics by hydrazine and the decomposition of hydrazine. *Fuel*, vol. 84, pp. 1-4, 2005.

#### Coal conversion

1. Johnson, B.C., M.M. Fegley, and H.H. Schobert, The Grand Forks slagging gasifier, *Coal Processing Technology*, vol. 4, pp. 94-98, 1978.
2. Miller, D.J., J.K. Olson, and H.H. Schobert, Mass spectroscopic characterization of tars from the gasification of low-rank coals, *Fuel*, vol. 60, pp. 369-374, 1981.
3. Garcia, A.B. and H.H. Schobert, Hydrodesulfurization of Spanish lignite with a high organic sulfur content, *Coal Preparation*, vol. 7, pp. 47-54, 1989.
4. Garcia, A.B. and H.H. Schobert, Effects of organic sulfur content on thermolysis and hydrogenolysis of lignites, *Fuel Processing Technology*, vol. 24, pp. 179-186, 1990.
5. Garcia, A.B. and H.H. Schobert, Catalytic hydrodesulfurization of a high organic sulfur Turkish lignite: amount, form, and mechanism of sulfur removal. *Fuel Processing Technology*, vol. 26, pp. 99-110, 1990.
6. Burgess, C.E. and H.H. Schobert, Behavior of tetrahydroquinoline in temperature-staged liquefaction of subbituminous coal, *Fuel*, vol. 70, pp. 372-379, 1991.
7. Chamberlin, P.L. and H.H. Schobert, Effect of mobile phase and network properties on liquefaction behavior of bituminous coals, *Fuel Processing Technology*, vol. 28, pp. 67-76, 1991.
8. Eser, S., R.G. Jenkins, G. Wei, H.H. Schobert, and J.T. Joseph, High-temperature swelling of coal/tetralin mixtures in a high-pressure microdilatometer, *Fuel*, vol. 70, pp. 1445-1455, 1991.
9. Garcia, A.B. and H.H. Schobert, Hydrodesulfurization of a high organic sulfur Spanish lignite with impregnated nickel sulfate, *Coal Preparation*, vol. 9, pp. 185-197, 1991.

10. Schobert, H.H. and A.B. Garcia, Liquefaction behavior of high-sulfur lignites, In: *Coal Science II*, Schobert, H.H., K.D. Bartle, and L.J. Lynch, Eds., American Chemical Society, Washington, Chapter 16, 1991.
11. Solomon, P.R., M.A. Serio, G.V. Deshpande, E. Kroo, H.H. Schobert, and C.E. Burgess, An investigation of the chemistry of preliquefaction, In: *Coal Science II*, Schobert, H.H., K.D. Bartle, and L.J. Lynch, Eds., American Chemical Society, Washington, Chapter 15, 1991.
12. Artok, L., A. Davis, G.D. Mitchell, and H.H. Schobert, Swelling pretreatment of coals for improved liquefaction, *Fuel*, vol. 71, pp. 981-991, 1992.
13. Artok, L., A. Davis, and H.H. Schobert, Temperature-staged liquefaction of coals impregnated with ferrous sulfate, *Fuel Processing Technology*, vol. 32, pp. 87-100, 1992.
14. Song, C., H.H. Schobert, and P.G. Hatcher, Temperature-programmed liquefaction of low-rank coal, *Energy and Fuels*, vol. 6, pp. 326-328, 1992.
15. Artok, L., A. Davis, G.D. Mitchell, and H.H. Schobert, Swelling pretreatment of coals for improved catalytic temperature-staged liquefaction, *Energy and Fuels*, vol. 7, pp. 67-77, 1993.
16. Saini, A.K., M.M. Coleman, C. Song, and H.H. Schobert, Antiliquefaction: model systems for enhanced retrogressive crosslinking reactions under coal liquefaction conditions, *Energy and Fuels*, vol. 7, pp. 328-330, 1993.
17. Song, C., L. Hou, A.K. Saini, P.G. Hatcher, and H.H. Schobert, CPDAS <sup>13</sup>C NMR and pyrolysis-GC-MS studies of structure and liquefaction reactions of Montana subbituminous coal, *Fuel Processing Technology*, vol. 34, pp. 249-276, 1993.
18. Tomic, J. and H.H. Schobert, Comparative reactivity of caking and non-caking coals under coprocessing conditions, *Fuel Processing Technology*, vol. 34, pp. 295-312, 1993.
19. Song, C., A.J. Saini, and H.H. Schobert. Effects of drying and oxidation of Wyodak subbituminous coal on its thermal and catalytic liquefaction. Spectroscopic characterization and products distribution. *Energy and Fuels*, vol. 8, pp. 301-312, 1994.
20. Artok, L., H.H. Schobert, and O. Erbatur. Temperature-staged liquefaction of selected Turkish coals, *Fuel Processing Technology*, vol. 37, pp. 211-236, 1994.
21. Dutta, R. and H.H. Schobert. Dammar resin: A chemical model for reactions of Utah resinite. In: *Amber, Resinite, and Fossil Resins*, Anderson, K.B. and J.C. Crelling, Eds., American Chemical Society, Washington, Chapter 15, 1995.
22. Tomic, J. and H.H. Schobert. Coal conversion with selected model compounds under noncatalytic, low solvent:coal ratio conditions. *Energy and Fuels*, vol. 10, pp. 709-717, 1996.
23. Burgess, C.E. and H.H. Schobert. Effect of coal characteristics and molybdenum sulfide catalyst on conversions and yields of heavy products from liquefaction in phenanthrene. *Energy and Fuels*, vol. 10, pp. 718-725, 1996.
24. Artok, L., O. Erbatur, and H.H. Schobert. Reactions of dinaphthyl and diphenyl ethers at liquefaction conditions. *Fuel Processing Technology*, vol. 47, pp. 153-176, 1996.



25. Tomic, J. and H.H. Schobert. Coal/petroleum residuum interactions during coprocessing under noncatalytic, low solvent/coal ratio conditions. *Energy and Fuels*, vol. 11, pp. 116-125, 1997.
26. Artok, L., Schobert, H.H., Nomura, M., Erbatur, O., and K. Kidena. Effects of water and molecular hydrogen on heat treatment of Turkish low-rank coals. *Energy and Fuels*, vol. 12, pp. 1200-1211, 1998.
27. Burgess, C.E. and H.H. Schobert. Relationship of coal characteristics determined by pyrolysis /gas chromatography/mass spectrometry and nuclear magnetic resonance to liquefaction reactivity and product composition. *Energy and Fuels*, vol. 12, pp. 1212-1222, 1998.
28. Tomic, J., and H.H. Schobert. Retrogressive reactions in non-catalytic coprocessing of coal and petroleum residua. *Hemijaska Industrija*, vol. 52, pp. 239-247, 1998.
29. Artok, L. and H.H. Schobert. Reaction of carboxylic acids under coal liquefaction conditions. 1. Under nitrogen atmosphere. *Journal of Analytical and Applied Pyrolysis*. vol. 54, pp 215-234, 2000.
30. Artok, L. and H.H. Schobert. Reaction of carboxylic acids under coal liquefaction conditions. 2. Under hydrogen atmosphere. *Journal of Analytical and Applied Pyrolysis*. vol. 54, pp 235-246, 2000.
31. Korda, A., Larsen, J.W., Martin, S.C., Saini, A.K., Schobert, H.H., and C. Song. Nonradical reactions during coal conversion. A search for synchronous 1,4-hydrogen addition as a precursor to radical reactions. *Energy and Fuels*, vol. 14, pp. 545-551. 2000.
32. Fickinger, A.E., M.W. Badger, G.D. Mitchell, and H.H. Schobert. Laboratory-scale coking of coal-petroleum mixtures in sealed reactors. *Energy and Fuels*, vol. 18, pp. 976-986, 2004.
33. Andrésen, J.M., Y. Zhang, C.E. Burgess and H.H. Schobert. Synthesis of pitch materials from hydrogenation of anthracite. *Fuel Processing Technology*, vol. 85, pp. 1361-1372, 2004.
34. Huang, L. and H.H. Schobert. Comparison of temperature conditions in direct liquefaction of selected low-rank coals. *Energy and Fuels*, vol. 19, pp. 200-207, 2005.
35. Jusino, A., and H.H. Schobert. The use of sulfur to extract hydrogen from coal. *International Journal of Coal Geology*, vol. 65, pp. 223-234, 2006.
36. Gül, O., L.R. Rudnick, and H.H. Schobert. Delayed coking of decant oil and coal in a laboratory-scale coking unit. *Energy and Fuels*, vol. 20, pp. 1647-1655, 2006.
37. Gül, O., P. Gafarova, A. Hesenov, H.H. Schobert, and O. Erbatur. Catalytic direct liquefaction of high-sulfur coals and their blends with asphaltite in the absence of a solvent. *Energy and Fuels*. vol. 21, pp. 2216-2225, 2007.
38. Skhonde, M.P., R.H. Matjie, J.R. Bunt, C.A. Strydom, and H.H. Schobert. Sulfur behavior in the Sasol-Lurgi fixed-bed dry-bottom gasification process. *Energy and Fuels*, vol. 23, pp. 229-235, 2009.

39. Gl, O., C.E.B. Clifford, L.R. Rudnick, and H.H. Schobert. Characterization of liquids derived from laboratory coking of decant oil and co-coking of Pittsburgh seam bituminous coal with decant oil. *Energy and Fuels*, vol. 23, pp. 2637-2645, 2009.
40. Clifford, C.E.B., H.H. Schobert, J.M. Griffith, and L.R. Rudnick. Solvent extraction of bituminous coals using light cycle oil: characterization of diaromatic products in liquids. *Energy and Fuels*, vol. 23, pp. 4553-4561, 2009.
41. Wang, S., Y. Tang, H.H. Schobert, Q. Guo, and F. Wang. Liquefaction reactivity and <sup>13</sup>C NMR of coals rich in barkinite and semifusinite. *Journal of Fuel Chemistry and Technology*, vol. 38, pp. 129-133, 2010.
42. Skhonde, M.P., C.A. Strydom J.R. Bunt, and H.H. Schobert. Sulphur capturing by inertinite-rich high-ash bituminous coal during conversion in a pilot packed bed. *Journal of Analytical and Applied Pyrolysis*, vol. 91, pp. 205-209, 2011.
43. Bunt, J.R., F.B. Waanders, and H.H. Schobert. Behaviour of selected major elements during fixed-bed gasification of South African bituminous coal. *Journal of Analytical and Applied Pyrolysis*, vol. 93, pp. 85-94, 2012.
44. Wang, S., Y. Tang, H.H. Schobert, Y. Guo, and Y. Su. Petrology and structural studies in liquefaction reactions of Late Permian coals from southern China. *Fuel*, vol. 107, pp. 518-524, 2013.
45. Schobert, H.H. Toward the zero-emission coal-to-liquids plant. *Technology*, 2015 (on line ready).

#### Fuel cells

1. Zhou, Z.F., C. Gallo, M.B. Pague, H.H. Schobert, and S.N. Lvov. Direct oxidation of jet fuels and Pennsylvania crude oil in a solid oxide fuel cell. *Journal of Power Sources*. vol. 133, pp. 181-187, 2004.
2. Zhou, Z.F., R. Kumar, S.T. Thakur, L.R. Rudnick, H.H. Schobert, and S.N.Lvov. Direct oxidation of waste vegetable oil in solid oxide fuel cells. *Journal of Power Sources*. vol. 171, pp. 856-860, 2007.

#### Geochemistry and structure of coals

1. Karner, F.R., S.A. Benson, H.H. Schobert, and R.G. Roaldson, Geochemical variation of inorganic constituents in a North Dakota lignite, In: *The Chemistry of Low-Rank Coals*, Schobert, H.H. (Ed.), American Chemical Society, Washington, Chapter 11, 1984.
2. Karner, F.R., H.H. Schobert, S.K. Falcone, and S.A. Benson, Elemental distribution and association with inorganic and organic components in North Dakota lignites, In: *Mineral Matter and Ash in Coal*, Vorres, K.S. (Ed.), American Chemical Society, Washington, Chapter 6, 1986.
3. Schobert, H.H., The geochemistry of coal. I. The classification and origin of coal, *Journal of Chemical Education*, vol. 66, pp. 242-244, 1989.
4. Schobert, H.H., The geochemistry of coal. II. The components of coal, *Journal of Chemical Education*, vol. 66, pp. 290-294, 1989.

5. Wang, S., Y. Tang, H.H. Schobert, G.D. Mitchell, F. Liao, and Z. Liu. A thermal behavior study of Chinese coals with high hydrogen content. *International Journal of Coal Geology*, vol. 81, pp. 37-44, 2010.
6. Mathews, J.P., V. Fernandez-Alos, A.D. Jones, and H.H. Schobert. Determining the molecular weight distribution of Pocahontas No. 3 low-volatile bituminous coal utilizing HRTWM and laser desorption ionization mass spectra data. *Fuel*, vol. 89, pp. 1461-1469, 2010.
7. Wang, S., Y. Tang, H.H. Schobert, Y. Guo, and Y. Su. FTIR and <sup>13</sup>C NMR investigation of coal components of late Permian coals from southern China. *Energy and Fuels*, vol. 25 pp. 5672-5677, 2011.
8. Strydom, C.A., J.R. Bunt, H.H. Schobert, and M. Raghoo. Changes to the organic functional groups of an interinite-rich medium-rank bituminous coal during acid treatment processes. *Fuel Processing Technology*, vol. 92, pp. 764-770, 2011.
9. Wang, S., Y. Tang, H.H. Schobert, Y. Guo, W. Guo, and X. Lu. FTIR and simultaneous TG/MS/FTIR study of Late Permian coal from southern China. *Journal of Analytical and Applied Pyrolysis*, vol. 100, pp. 75-80, 2013.
10. Wang, S., Y. Tang, H.H. Schobert, D. Jiang, X. Guo, F. Huang, Y. Guo, and Y. Su. Chemical compositional and structural characterization of Late Permian bark coals from southern China, *Fuel*, vol. 126, p. 116-121, 2014.

#### Graphite

1. Jiang, Y.J., M.S. Solum, R.J. Pugmire, D.M. Grant, H.H. Schobert, and P.J. Pappano. A new method for measuring the graphite content of anthracite coals and soots. *Energy and Fuels*, vol. 16, pp. 1296-1300, 2002.
2. Atria, J.V., F. Rusinko Jr., and H.H. Schobert. Structural ordering of Pennsylvania anthracites on heat treatment to 2000–2900°C. *Energy and Fuels*, vol. 16, pp. 1343-1347, 2002.
3. Pappano, P.J., F. Rusinko, H.H. Schobert, and D.P. Struble. Dependence of physical properties of isostatically molded graphites on crystalline height. *Carbon*. vol. 42, pp. 3007-3009, 2004.
4. Pappano, P.J. and H.H. Schobert. Effect of natural mineral inclusions on the graphitizability of a Pennsylvania anthracite. *Energy and Fuels*, vol. 23, pp. 422-428, 2009.
5. Nyathi, M.S., C.B. Clifford, and H.H. Schobert. Characterization of graphitic materials prepared from different rank Pennsylvania anthracites. *Fuel*, vol. 114, pp. 244-255, 2013.

#### High-temperature physical chemistry of aluminosilicate ashes and slags

1. Schobert, H.H. and C. Witthoeft, The petrochemistry of coal ash slags. 3. Petro-chemical behavior of the Rosebud slag–limestone system, *Fuel Processing Technology*, vol. 5, pp. 157-164, 1981.
2. Streeter, R.C., E.K. Diehl, and H.H. Schobert, Measurement and prediction of low-rank coal slag viscosity, In: *The Chemistry of Low-Rank Coals*, Schobert, H.H. (Ed.), American Chemical Society, Washington, Chapter 12, 1984.

3. Schobert, H.H., R.C. Streeter, and E.K. Diehl, The flow properties of low-rank coal ash slags: implications for slagging gasification. *Fuel*, vol. 64, pp. 1611-1617, 1985.
4. Falcone, S.K. and H.H. Schobert, Mineral transformations during ashing and slagging of selected low-rank coals, In: *Mineral Matter and Ash in Coal*, Vorres, K.S. (Ed.), American Chemical Society, Washington, Chapter 9, 1986.
5. Jung, B.J. and H.H. Schobert, Viscous sintering of coal ashes. 1. Relationships of sinter point and sinter strength to particle size and composition, *Energy and Fuels*, vol. 5, pp. 555-561, 1991.
6. Hurley, J.P. and H.H. Schobert, Ash formation during pulverized subbituminous coal combustion. 1. Characterization of coals, and inorganic transformations during early stages of burnout, *Energy and Fuels*, vol. 6, pp. 47-58, 1992.
7. Jung, B.J. and H.H. Schobert, Viscous sintering of coal ashes. 2. Sintering behavior at short residence times in a drop tube furnace, *Energy and Fuels*, vol. 6, pp. 59-68, 1992.
8. Jung, B.J. and H.H. Schobert, Improved prediction of coal ash slag viscosity by thermodynamic modeling of liquid-phase composition, *Energy and Fuels*, vol. 6, pp. 387-398, 1992.
9. Miller, S.F. and H.H. Schobert, Effect of fuel particle and droplet size distribution on particle size distribution of char and ash during pilot-scale combustion of pulverized coal and coal-water slurry fuels, *Energy and Fuels*, vol. 7, pp. 520-531, 1993.
10. Miller, S.F. and H.H. Schobert, Effect of mineral matter particle size on ash particle size distribution during pilot-scale combustion of pulverized coal and coal-water slurry fuels, *Energy and Fuels*, vol. 7, pp. 532-541, 1993.
11. Hurley, J.P. and H.H. Schobert, Ash formation during pulverized subbituminous coal combustion. 2. Inorganic transformations during middle and late stages of burnout, *Energy and Fuels*, vol. 7, pp. 542-553, 1993.
12. Miller, S.F. and H.H. Schobert. Effects of the occurrence and composition of iron compounds on ash formation, composition, and size in pilot-scale combustion of pulverized coal and coal-water slurry fuels. *Energy and Fuels*, vol. 7, pp. 1030-1038, 1993.
13. Miller, S.F. and H.H. Schobert. Effect of the occurrence and composition of silicate and aluminosilicate compounds on ash formation in pilot-scale combustion of pulverized coal and coal-water slurry fuels. *Energy and Fuels*, vol. 8, pp. 1197-1207, 1994.
14. Miller, S.F. and H.H. Schobert. Effect of the occurrence and modes of incorporation of alkalis, alkaline earth elements, and sulfur on ash formation in pilot-scale combustion of Beulah pulverized coal and coal-water slurry fuel. *Energy and Fuels*, vol. 8, pp. 1208-1216, 1994.
15. Shamanna, S. and H.H. Schobert. Fireside corrosion of selected alloys by ash recovered from coal-water slurry combustion. *Fuel Processing Technology*, vol. 53, pp. 133-156, 1998.
16. Folkedahl, B.C. and H.H. Schobert. Effects of atmosphere on viscosity of selected bituminous and low-rank coal ash slags, *Energy and Fuels*, vol. 19, pp. 208-215, 2005.

17. Moitsheki, L.J., R.H. Matjie, and H.H. Schobert. Chemical and mineralogical characterization of a South African bituminous coal and its ash, and effect on pH of ash transport water. *Minerals Engineering*, vol. 23, pp. 258-261, 2010.
18. Nel, M.V., C.A. Strydom, H.H. Schobert, J.P. Beukes, and J.R. Bunt. Comparison of sintering and compressive strength tendencies of a model coal mineral mixture heat treated in inert and oxidizing atmospheres. *Fuel Processing Technology*, vol. 92, pp. 1042-1051, 2011.
19. Nel, M.V., C.A. Strydom, H.H. Schobert, J.P. Beukes, and J.R. Bunt. Reducing atmosphere ash fusion temperatures of a mixture of coal-associated minerals—The effect of inorganic additives and ashing temperature. *Fuel Processing Technology*, vol. 124, pp. 78-86, 2014.
20. Nel, M.V., C.A. Strydom, H.H. Schobert, J.P. Beukes, and J.R. Bunt. Effect of sodium compounds on the sintering propensity of coal-associated minerals. *Journal of Analytical and Applied Pyrolysis*, vol. 111, pp. 94-99, 2015.

#### Jet fuel from coal

1. Coleman, M.M., H.H. Schobert, and C. Song. A new generation of jet fuels. *Chemistry in Britain*, vol. 29, pp. 760-762, 1993.
2. Burgess, C.E. and H.H. Schobert. Direct liquefaction for production of high yields of feedstocks for specialty chemicals or thermally stable jet fuels. *Fuel Processing Technology*, vol. 64, pp. 57-72, 2000.
3. Gül, O., L.R. Rudnick, and H.H. Schobert. The effect of chemical composition of coal-based jet fuels on the deposit tendency and morphology. *Energy and Fuels*, vol. 20, pp. 2478-2485, 2006.
4. Gül, O., L.R. Rudnick, and H.H. Schobert. Effect of the reaction temperature and fuel treatment on the deposit formation of jet fuels. *Energy and Fuels*, vol. 22, pp. 433-439, 2008.
5. Balster, L.M., E. Corporan, M.J. DeWitt, J.T. Edwards, J.S. Ervin, J.L. Graham, S.Y. Lee, S. Pal, D.K. Phelps, L.R. Rudnick, R.J. Santoro, H.H. Schobert, L.M. Shafer, R.C. Striebich, Z.J. West, G.R. Wilson, R. Woodward, and S. Zabarnick. Development of an advanced, thermally stable, coal-based jet fuel. *Fuel Processing Technology*, vol. 89, pp. 364-378, 2008.

#### Molecular modeling and theoretical chemistry

1. Schobert, H.H., A magnetic analogy for demonstrating some VSEPR principles, *Journal of Chemical Education*, vol. 50, p. 651, 1973.
2. Ma, X., Wang, Q., Chen, L.Q., Cermignani, W., Schobert, H.H., and C.G. Pantano. Semi-empirical studies on electronic structures of a boron-doped graphene layer—implications on the oxidation mechanism. *Carbon*, vol. 35, pp. 1517-1525, 1997.
3. Song, C., Ma, X., and H.H. Schobert. Computational analysis for shape-selective alkylation of naphthalene over zeolite catalysts. In: *Shape-Selective Catalysis*. Song, C.,

Garcés, J.M., and Sugi, Y. (Eds.) American Chemical Society: Washington, 2000; Chapter 22.

4. Ma, X. and H.H. Schobert. Estimating heats of formation of hydrocarbon radicals by a combination of semiempirical calculation and family correlation with experimental values. *Journal of Physical Chemistry A*, vol. 104, pp. 1064-1074, 2000.
5. Ma, X., and H.H. Schobert. Molecular simulation of hydrodesulfurization of thiophenic compounds over MoS<sub>2</sub> using ZINDO. *Journal of Molecular Catalysis A: Chemical*, vol. 160, pp. 409-427, 2000.
6. Ma, X. and H.H. Schobert. Estimating the activation energy for hydrogen abstraction reactions by a combination of semiempirical calculation and family correlations. *Industrial and Engineering Chemistry Research*, vol. 40, pp. 743-750, 2001.
7. Ma, X. and H.H. Schobert. Estimating the activation energy of hydrogen abstraction reactions involving hydrocarbons by thermochemical properties. *Industrial and Engineering Chemistry Research*, vol. 42, pp. 1151-1161, 2003.

#### Petroleum processing

1. Escallon, M.M., D.A. Fonseca, and H.H. Schobert. Characterization of hydrotreated decant oils. Effect of different severities of hydroprocessing on decant oil chemical composition. *Energy and Fuels*, vol. 27, pp. 478-486, 2013.

#### Pyrolysis, thermal decomposition, and carbonization

1. Bale, H.D., M.L. Carlson, and H.H. Schobert, Thermal modification of the pore structure of a North Dakota lignite, *Fuel*, vol. 65, pp. 1185-1189, 1986.
2. Hefta, R.S., H.H. Schobert, and W.R. Kube, Calorimetric pyrolysis of a North Dakota lignite, *Fuel*, vol. 65, pp. 1196-1202, 1986.
3. Lee, C.W., R.G. Jenkins, and H.H. Schobert. Mechanisms and kinetics of rapid, elevated pressure pyrolysis of Illinois No. 6 bituminous coal, *Energy and Fuels*, vol. 5, pp. 547-555, 1991.
4. Lee, C.W., R.G. Jenkins and H.H. Schobert, Structure and reactivity of char from elevated pressure pyrolysis of Illinois No. 6 bituminous coal, *Energy and Fuels*, vol. 6, pp. 40-47, 1992.
5. Song, C., S. Eser, H.H. Schobert, and P.G. Hatcher, Pyrolytic degradation studies of a coal-derived and a petroleum-derived aviation jet fuel, *Energy and Fuels*, vol. 7, pp. 234-243, 1993.
6. Sasaki, T., R.G. Jenkins, S. Eser, and H.H. Schobert. Carbonization of anthracene and phenanthrene. 1. Kinetics and mesophase development. *Energy and Fuels*, vol. 7, pp. 1039-1046, 1993.
7. Sasaki, T., R.G. Jenkins, S. Eser, and H.H. Schobert. Carbonization of anthracene and phenanthrene. 2. Spectroscopy and mechanisms. *Energy and Fuels*, vol. 7, pp. 1047-1053, 1993.
8. Song, C., W.C. Lai, and H.H. Schobert. Condensed-phase pyrolysis of *n*-tetradecane at elevated pressures for long duration. Product distribution and reaction mechanisms. *Industrial and Engineering Chemistry Research*, vol. 33, pp. 534-547, 1994.

9. Song, C., W.C. Lai, and H.H. Schobert. Hydrogen-transferring pyrolysis of long-chain alkanes and thermal stability improvement of jet fuels by hydrogen donors. *Industrial and Engineering Chemistry Research*, vol. 33, pp. 548-557, 1994.
10. Nyathi, M.S., C.B. Clifford, and H.H. Schobert. Effect of petroleum feedstock and reaction conditions on the structure of coal-petroleum co-cokes and heat-treated products. *Energy and Fuels*, vol. 26, pp. 4413-4419, 2012.
11. Gül, O., L.R. Rudnick, and H.H. Schobert. Co-coking of hydrotreated decant oil/coal blends: Effect of hydrotreatment severity on the yield distribution and quality of distillable fuels. *Energy and Fuels*, vol. 27, pp. 3071-3079, 2013.
12. Coetzee, S., H.W.J.P. Neomagus, J.R. Bunt, C.A. Strydom, and H.H. Schobert. The transient swelling behavior of large South African coal particles during low temperature devolatilization. *Fuel*, vol. 136, pp. 79-88, 2014.
13. Coetzee, S., H.W.J.P. Neomagus, J.R. Bunt, J.P. Mathews, C.A. Strydom, and H.H. Schobert. Reduction of caking propensity in large South African coal particles with potassium carbonate impregnation to expand fixed- and fluidized-bed gasification feedstock suitability. *Energy and Fuels*, 2015, DOI 10.1021/acs.energyfuels.5b00C74.

## Reviews

1. Kube, W.R., H.H. Schobert, S.A. Benson, and F.R. Karner, Some aspects of the structure and reactions of northern Great Plains lignites, In: *The Chemistry of Low-Rank Coals*, Schobert, H.H. (Ed.), American Chemical Society, Washington, Chapter 3, 1984.
2. Schobert, H.H., F.R. Karner, E.S. Olson, D.R. Kleesattel, and C.J. Zygarlicke, New approaches to the characterization of lignites: a combined geological and chemical study, In: *Coal Science and Chemistry*, Volborth, A. (Ed.), Elsevier, Amsterdam, Chapter 14, 1987.
3. Schobert, H.H., Structural features of low-rank coals, *Resources, Recovery and Recycling*, vol. 3, pp. 111-123, 1990.
4. Song, C. and H.H. Schobert, Opportunities for developing specialty chemicals and advanced materials from coal, *Fuel Processing Technology*, vol. 34, pp. 157-196, 1993.
5. Song, C. and H.H. Schobert. Non-fuel uses of coals and synthesis of chemicals and materials. *Fuel*, vol. 75, pp. 724-736, 1996.
6. Schobert, H.H. and C. Song. Chemicals and materials from coal in the 21st century. *Fuel*, vol. 81, pp. 15-32, 2002.
7. Andrésen, J.M., C.E. Burgess, P.J. Pappano, and H.H. Schobert. New directions for non-fuel uses of anthracite. *Fuel Processing Technology*. vol. 85, pp. 1373-1392, 2004.
8. Mathews, J.P., B.G. Miller, C. Song, H.H. Schobert, F. Botha, and R.B. Finkleman. The ebb and flow of U.S. coal research 1970–2010 with a focus on academic institutions. *Fuel*, vol. 105, pp. 1-12, 2013.
9. Schobert, H.H. Production of acetylene and acetylene-based chemicals from coal. *Chemical Reviews*, vol. 114, pp. 1743-1760, 2014.

