

## **Jonathan P. Mathews, Ph.D.**

Coal Scientist, The Pennsylvania State University, 126 Hosler Building  
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### **Professional Preparation**

The Nottingham Trent University, UK Applied Chemistry B.Sc. (Hons), 1991  
The Pennsylvania State University, Fuel Science Ph.D., 1998

### **Appointments**

July 2016 – Current Professor of Energy & Mineral Engineering, The Pennsylvania State University (tenured)  
July 2013 – June 2016 Associate Professor of Energy & Mineral Engineering, The Pennsylvania State University (tenured)  
July 2008 – June 2013 Assistant Professor of Energy & Mineral Engineering, The Pennsylvania State University (tenure track)  
July 2000 – June 2008 Assistant Professor of Energy & Geo-Environmental Engineering, The Pennsylvania State University  
June 1998 – June 2000, Research Associate, The Energy Institute & The Energy & Geo-Environmental Engineering Department, The Pennsylvania State University

### **Summary**

A coal scientist, ~95 peer-reviewed journal articles, 2 book chapters, 85 conference papers, graduated 5 Ph.D. and 7 M.S. students.

### **Graduate Advisors**

Alan W. Scaroni (retired), Pennsylvania State University & Patrick Hatcher (currently at Old Dominion).

### **Publications**

#### *Peer-reviewed journal articles*

- 1 S. Yu, J. Bo, V. Vandeginste, J.P. Mathews, Deformation-related coalification: Significance for deformation within shallow crust, *International Journal of Coal Geology*, (2022).
- 2 Y. Du, C.a. Wang, D. Che, J.P. Mathews, The influence of char particle morphology on char burnout behavior by atomistic simulation, *Fuel*, 314 (2022).
- 3 Y. Zhang, S. Hu, Q. Zhong, J. Zhuo, J.P. Mathews, A large-scale molecular model of Fenghuangshan anthracite coal, *Fuel*, 295 (2021).
- 4 L. Yuan, Q. Liu, J.P. Mathews, H. Zhang, Y. Wu, Quantifying the structural transitions of Chinese coal to coal-derived natural graphite by XRD, Raman spectroscopy, and HRTEM image analyses, *Energy & Fuels*, 35 (2021) 2335-2346.
- 5 X. Wang, Y. Zhu, S. Chen, X. Dai, Q. Xu, Y. Song, J.P. Mathews, Molecular structure evaluation and image-guided atomistic representation of marine kerogen from Longmaxi Shale, *Energy & Fuels*, (2021).
- 6 W. Li, Y. Song, W.-b. Yang, J.P. Mathews, Structural transformations for a subbituminous coal, impact of temperature on gold-tube pyrolysis chars evaluated using HRTEM, *Fuel*, 311 (2021).

- 7 S. Chen, D. Tang, S. Tao, P. Liu, J.P. Mathews, Implications of the in situ stress distribution for coalbed methane zonation and hydraulic fracturing in multiple seams, western Guizhou, China, *Journal of Petroleum Science and Engineering*, 204 (2021).
- 8 X. Wang, Y. Zhu, Y. Song, J.P. Mathews, Structure and partial ordering of terrestrial kerogen: Insight from high-resolution transmission electron microscopy, *Fuel*, 281 (2020).
- 9 Y. Song, B. Jiang, M. Li, C.L. Hou, J.P. Mathews, Macromolecular transformations for tectonically-deformed high volatile bituminous via HRTEM and XRD analyses, *Fuel*, 263 (2020).
- 10 Y.L. Liu, H. Xu, D.Z. Tang, F.Y. Xu, J.P. Mathews, W. Hou, X. Yan, F.F. Ding, Coalbed methane production of a heterogeneous reservoir in the Ordos Basin, China, *J Nat Gas Sci Eng*, 82 (2020).
- 11 Q.H. Chang, R. Gao, M. Gao, G.S. Yu, J.P. Mathews, F.C. Wang, Experimental analysis of the evolution of soot structure during CO<sub>2</sub> gasification, *Fuel*, 265 (2020).
- 12 Q. Zhong, Y. Zhang, S. Shabnan, Q. Mao, J. Xiao, A.C.T. Van Duin, J.P. Mathews, ReaxFF MD simulations of petroleum coke CO<sub>2</sub> gasification examining the S/N removal mechanisms and CO/CO<sub>2</sub> reactivity, *Fuel*, 257 (2019).
- 13 Q. Zhong, Y. Zhang, S. Shabnam, J. Xiao, A.C.T. van Duin, J.P. Mathews, Reductive gaseous (H<sub>2</sub>/NH<sub>3</sub>) desulfurization and gasification of high-sulfur petroleum coke via reactive force field molecular dynamics simulations, *Energy Fuels*, 33 (2019) 8065-8075.
- 14 Y. Zhang, X. Zhang, Q. Zhong, S. Hu, J.P. Mathews, Structural differences of spontaneous combustion prone inertinite-rich Chinese lignite coals: Insights from XRD, Solid-State <sup>13</sup>C NMR, LDIMS, and HRTEM, *Energy Fuels*, 33 (2019) 4575-4584.
- 15 Y. Du, C. Wang, H. Xin, J.P. Mathews, Competitive or additive behavior for H<sub>2</sub>O and CO<sub>2</sub> gasification of coal char? Exploration via simplistic atomistic simulation, *Carbon*, 141 (2019) 226-237.
- 16 Y. Du, C. Wang, H. Xin, D. Che, J.P. Mathews, Atomistic simulation of coal char oxy-fuel combustion: quantifying the influences of CO<sub>2</sub> to char reactivity, *Energy Fuels*, 33 (2019) 10228-10236.
- 17 Q. Zhong, Q. Mao, L. Zhang, J. Xiang, J. Xiao, J.P. Mathews, Structural features of Qingdao petroleum coke from HRTEM lattice fringes: Distributions of length, orientation, stacking, curvature, and a large-scale image-guided 3D atomistic representation, *Carbon*, 129 (2018) 790-802.
- 18 Q. Zhong, Q. Mao, J. Xiao, A. van Duin, J.P. Mathews, ReaxFF simulations of petroleum coke sulfur removal mechanisms during pyrolysis and combustion *Combustion and Flame*, 198 (2018) 146-157.
- 19 Q. Zhong, Q. Mao, J. Xiao, A. van Duin, J.P. Mathews, Sulfur removal from petroleum coke during high-temperature pyrolysis. analysis from TG-MS data and ReaxFF simulations, *Journal of Analytical and Applied Pyrolysis*, 132 (2018) 134-142.
- 20 C. Wang, T. Huddle, C.-H. Huang, W. Zhu, R.L. Vander Wal, E. Lester, J.P. Mathews, Improved quantification of curvature in high-resolution transmission electron microscopy lattice fringe micrographs of soots, *Carbon*, 117 (2017) 174-181.

- 21 Y. Song, B. Jiang, J.P. Mathews, G. Yan, F. Li, Structural transformations and hydrocarbon generation of low-rank coal (vitrinite) during slow heating pyrolysis, *Fuel Processing Technology*, 167 (2017) 535-544.
- 22 J.P. Mathews, Q.P. Campbell, H. Xu, P. Halleck, Application of X-ray computed tomography to the study of coal *Fuel*, 209 (2017) 10-24.
- 23 G.H. Coetzee, R. Sakurovs, H.W.J.P. Neomagus, R. Everson, J.P. Mathews, J.R. Bunt, Particle size influence on the pore development of nanopores in coal gasification chars: from micron to millimeter particles, *Carbon*, 112 (2017) 37-46.
- 24 J.P. Abrahamson, M. Singh, J.P. Mathews, R.L. Vander Wal, Pulsed laser annealing of carbon black, *Carbon*, 124 (2017) 380-390.
- 25 J. Zhao, H. Xu, D. Tang, J.P. Mathews, S. Li, S. Tao, A comparative evaluation of coal specific surface area by CO<sub>2</sub> and N<sub>2</sub> adsorption and its influence on CH<sub>4</sub> adsorption capacity at different pore sizes, *Fuel*, 183 (2016) 420-431.
- 26 J. Zhao, H. Xu, D. Tang, J.P. Mathews, S. Li, S. Tao, Coal seam porosity and fracture heterogeneity of macrolithotypes in the Hancheng Block, eastern margin, Ordos Basin, China, *International Journal of Coal Geology*, 159 (2016) 18-29.
- 27 H. Xu, D. Tang, J.P. Mathews, J. Zhao, B. Li, S. Tao, S. Li, Evaluation of coal macrolithotypes distribution by geophysical logging data in the Hancheng Block, Eastern Margin, Ordos Basin, China, *International Journal of Coal Geology*, 165 (2016) 265-277.
- 28 H. Xin, C. Wang, E. Louw, D. Wang, J.P. Mathews, Atomistic simulation of coal char isothermal oxy-fuel combustion: char reactivity and behavior, *Fuel*, 182 (2016) 935-943.
- 29 C. Wang, T. Huddle, E.H. Lester, J.P. Mathews, Quantifying curvature in HRTEM lattice fringe micrographs of coals, *Energy and Fuels*, 30 (2016) 2694-2704.
- 30 E. Louw, G.D. Mitchell, R.E. Winans, J.P. Mathews, Constitution of drop-tube generated coal chars from vitrinite-rich and inertinite-rich south African coals, *Energy Fuels*, 30 (2016) 112-120.
- 31 Y. Huang, F.S. Cannon, J. Guo, J.K. Watson, J.P. Mathews, Atomistic modeling insight into the structure of lignite-based activated carbon, and behavior of benzene sorption, *Rsc Adv*, 6 (2016) 56623-56637.
- 32 C. Wang, J.K. Watson, E. Louw, J.P. Mathews, A construction strategy for atomistic models of coal chars capturing stacking diversity and pore size distribution, *Energy Fuels*, 29 (2015) 4814-4826.
- 33 M.J. Roberts, R.C. Everson, H.W.J.P. Neomagus, D. Van Niekerk, J.P. Mathews, D.J. Branken, Influence of maceral composition on the structure, properties and behavior of chars derived from South African coals, *Fuel*, 142 (2015) 9-20.
- 34 M.J. Roberts, R.C. Everson, G. Domazetis, H.W.J.P. Neomagus, J.M. Jones, C.G.C.E. Van Sittert, G.N. Okolo, D.V. Niekerk, J.P. Mathews, Density functional theory molecular modelling and experimental particle kinetics for CO<sub>2</sub>-char gasification, *Carbon*, 93 (2015) 295-314.
- 35 M.A. Roberts, R.C. Everson, H.W.J.P. Neomagus, D. Van Niekerk, G.N. Okolo, J.P. Mathews, The characterisation of slow-heated inertinite- and vitrinite-rich coals from the South African coalfields, *Fuel*, 158 (2015) 591-601.
- 36 G.N. Okolo, H.W.J.P. Neomagus, R.C. Everson, M.J. Roberts, J.R. Bunt, R. Sakurovs, J.P. Mathews, Chemical-structural properties of South African bituminous coals: Insights

- from wide angle XRD-carbon fraction analysis, ATR-FTIR, solid state <sup>13</sup>C NMR, and HRTEM techniques, *Fuel*, 158 (2015) 779-792.
- 37 J.P. Mathews, C. Burgess-Clifford, P.C. Painter, The interactions of Illinois No. 6 bituminous coal with solvents: a review of solvent swelling and extraction literature, *Energy Fuels*, 29 (2015) 1279-1294.
- 38 H. Kumar, D. Elsworth, J.P. Mathews, C. Marone, Permeability evolution in sorbing media: analogies between organic-rich shale and coal, *Geofluids*, 133 (2015) 695-704.
- 39 H. Kumar, D. Elsworth, J.P. Mathews, Permeability evolution of propped artificial fractures in coals on injection of CO<sub>2</sub>, *Journal of Petroleum Science and Engineering*, 133 (2015) 695-704.
- 40 Y. Huang, F.S. Cannon, J.K. Watson, B. Reznik, J.P. Mathews, Activated carbon efficient atomistic model construction that depicts experimentally-determined characteristics, *Carbon*, 83 (2015) 1-14.
- 41 S. Coetzee, H.W.J.P. Neomagus, J.R. Bunt, J.P. Mathews, C.A. Strydom, H.H. Schobert, Reduction of caking propensity in large (mm sized) South African coal particles with potassium carbonate impregnation to expand fixed and fluidised bed gasification feedstock suitability, *Energy Fuels*, 29 (2015) 4255-4263.
- 42 G.H. Coetzee, R. Sakurovs, H.W.J.P. Neomagus, L. Morpeth, R. Everson, J.P. Mathews, J.R. Bunt, Pore development during gasification of South African inertinite-rich chars evaluated using small angle X-ray scattering, *Carbon*, 95 (2015) 250-260.
- 43 A. Tselev, I.N. Ivanov, N.V. Lavrik, A. Belianinov, S. Jesse, J.P. Mathews, G.D. Mitchell, S.V. Kalinin, Mapping internal structure of coal by confocal micro-Raman spectroscopy and scanning microwave microscopy, *Fuel*, 126 (2014) 32-37.
- 44 J.P. Mathews, V. Krishnamoorthy, E. Louw, A.H.N. Tchapda, F. Castro-Marcano, V. Karri, D.A. Alexis, G.D. Mitchell, A review of correlations of coal properties with elemental composition, *Fuel Processing Technology*, 121 (2014) 104-113.
- 45 H. Kumar, D. Elsworth, J.P. Mathews, J. Liu, D. Pone, Effect of CO<sub>2</sub> injection on heterogeneously permeable coalbed reservoirs, *Fuel*, 135 (2014) 509-521.
- 46 L. Collins, A. Tselev, S. Jesse, M.B. Okatan, R. Proksch, J.P. Mathews, G.D. Mitchell, B.J. Rodriguez, S.V. Kalinin, I.N. Ivanov, Breaking the limits of structural and mechanical imaging of the heterogeneous structure of coal macerals, *Nanotechnology*, 25 (2014) 435402.
- 47 F. Castro-Marcano, M.F. Russo, A.C.T. van Duin, J.P. Mathews, Pyrolysis of a large-scale molecular model of Illinois No. 6 coal using the ReaxFF reactive force field, *Journal of Analytical and Applied Pyrolysis*, 109 (2014) 79-89.
- 48 Y. Cai, D. Liu, J.P. Mathews, Z. Pan, D. Elsworth, Y. Yao, J. Li, X. Guo, Permeability evolution in fractured coal - combining triaxial confinement with X-ray computed tomography, acoustic emission and ultrasonic techniques, *International Journal of Coal Geology*, 122 (2014) 91-104.
- 49 E. Binner, E. Lester, S. Kingman, C. Dodds, J. Robinson, T. Wu, P. Wardle, J.P. Mathews, A review of microwave coal processing, *Journal of Microwave Power and Electromagnetic Energy*, 48 (2014) 35-60.
- 50 J.P. Mathews, B.G. Miller, C. Song, H.H. Schobert, F. Botha, R.B. Finkelman, The ebb and flow of U.S. coal research 1970-2010 with a focus on academic institutions, *Fuel*, 105 (2013) 1-12.

- 51 B.B. Hattingh, R.C. Everson, H.W.J.P. Neomagus, J.R. Bunt, D. Van Niekerk, J.H.L. Jordaan, J.P. Mathews, Elucidation of the structural and molecular properties of typical South African coals, *Energy and Fuels*, 27 (2013) 3161-3172.
- 52 Y.E. Alvarez, B.M. Moreno, M.T. Klein, J.K. Watson, F. Castro-Marcano, J.P. Mathews, A novel simplification approach for large-scale structural models of coal: 3D molecules to 2D lattices. 3. Reactive lattice simulations, *Energy and Fuels*, 27 (2013) 2915-2922.
- 53 R.L. Tolliver, J.P. Mathews, Reviews of science for science librarians: coal science and technology research 1970-2010, *Science & Technology Libraries*, 31 (2012) 146-163.
- 54 N. Pulati, M. Sobkowiak, J.P. Mathews, P. Painter, Low temperature treatment of Illinois No. 6 coal in ionic liquids, *Energy Fuels*, 26 (2012) 3548-3552.
- 55 J.O. Pou, Y.E. Alvarez, J.K. Watson, S. Pisupati, J.P. Mathews, Co-primary thermolysis molecular modeling simulation of lignin and subbituminous coal via a reactive coarse-grained simplification, *Journal of Analytical and Applied Pyrolysis*, 95 (2012) 101-111.
- 56 J.P. Mathews, A. Sharma, The structural alignment of coals and the analogous case of Argonne Upper Freeport Fuel, 95 (2012) 19-24.
- 57 J.P. Mathews, A. Chaffee, The molecular representations of coal — a review, *Fuel*, 96 (2012) 1-14.
- 58 H. Kumar, D. Elsworth, J.P. Mathews, J. Lui, D. Pone, Optimizing enhanced coalbed methane recovery for unhindered production and CO<sub>2</sub> injectivity, *International Journal of Greenhouse Gas Control*, 11 (2012) 86-97.
- 59 F. Castro-Marcano, R.E. Winans, P. Chupas, K. Chapman, J.M. Calo, J.K. Watson, J.P. Mathews, Fine structure evaluation of the pair distribution function with molecular models of the Argonne Premium coals, *Energy Fuels*, 26 (2012) 4336-4345.
- 60 F. Castro-Marcano, V.V. Lobodin, R.P. Rodgers, A.M. McKenna, A.G. Marshall, J.P. Mathews, A molecular model for the Illinois no. 6 Argonne Premium coal: moving towards capturing the continuum structure, *Fuel*, 95 (2012) 35-49.
- 61 F. Castro-Marcano, A.M. Kamat, M.F. Russo, A. van Duin, J.P. Mathews, Combustion of an Illinois No. 6 coal char simulated using an atomistic char representation and the ReaxFF reactive force field, *Combustion and Flame*, 159 (2012) 1272-1285.
- 62 Y.E. Alvarez, J.K. Watson, J.O. Pou, J.P. Mathews, A novel simplification approach for large-scale structural models of coal: 3D molecules to 2D lattices. 2. Visualization capabilities, *Energy Fuels*, 26 (2012) 4946-4952.
- 63 Y.E. Alvarez, J.K. Watson, J.P. Mathews, A novel simplification approach for large-scale structural models of coal: 3D molecules to 2D lattices. 1. Lattice creation, *Energy Fuels*, 26 (2012) 4938-4945.
- 64 D. Van Niekerk, J.P. Mathews, Molecular dynamics simulation of coal-solvent interactions in Permian-aged South African coals, *Fuel Processing Technology*, 92 (2011) 729-734.
- 65 D. Van Niekerk, F. Castro-Marcano, C.M. Colina, J.P. Mathews, Solvent swelling extent of Permian aged vitrinite- and inertinite-rich coals: experiments and modeling using perturbed-chain statistical associating fluid theory (PC-SAFT), *Energy Fuels*, 25 (2011) 2559-2564.

- 66 J.P. Mathews, A. van Duin, A. Chaffee, The utility of coal molecular models, *Fuel Processing Technology*, 92 (2011) 718-728.
- 67 J.P. Mathews, J.D.N. Pone, G.D. Mitchell, P. Halleck, High-resolution X-ray computed tomography observations of the thermal drying of lump-sized subbituminous coal, *Fuel Processing Technology*, 92 (2011) 58-64.
- 68 H. Kumar, E. Lester, S. Kingman, C. Avila, A. Jones, J. Robinson, P.M. Halleck, J.P. Mathews, Inducing fractures and increasing cleat apertures in bituminous coal under isostatic stress via application of microwave energy, *International Journal of Coal Geology*, 88 (2011) 75-82.
- 69 V. Fernandez-Alos, J.K. Watson, R. vander Wal, J.P. Mathews, Soot and char molecular representations generated directly from HRTEM lattice fringe images using Fringe3D, *Combustion and Flame*, 158 (2011) 1807-1813.
- 70 F. Castro-Marcano, J.P. Mathews, Constitution of Illinois No. 6 Argonne Premium coal: a review, *Energy Fuels*, 25 (2011) 845-853.
- 71 D. Van Niekerk, G.D. Mitchell, J.P. Mathews, Petrographic and reflectance analysis of solvent-swelled and solvent-extracted South African vitrinite-rich and inertinite-rich coals, *International Journal of Coal Geology*, 81 (2010) 45-52.
- 72 D. Van Niekerk, J.P. Mathews, Simulation of solvent extraction of South African vitrinite-rich and inertinite-rich coals, *Energy Fuels*, 24 (2010) 6393-6399.
- 73 D. Van Niekerk, J.P. Mathews, Molecular representations of vitrinite-rich and interinite-rich Permian aged South African coals, *Fuel*, 89 (2010) 73-82.
- 74 D. Van Niekerk, P. Halleck, J.P. Mathews, Solvent swelling behavior of Permian-aged South African vitrinite-rich and inertinite-rich coals, *Fuel*, 89 (2010) 19-25.
- 75 J.D.N. Pone, P.M. Halleck, J.P. Mathews, 3D characterization of strains in coal induced by compression, carbon dioxide sorption, and desorption at in situ stress conditions, *International Journal of Coal Geology*, 82 (2010) 262-268.
- 76 P. Painter, N. Pulati, R. Cetiner, M. Sobkowiak, G. Mitchell, J. Mathews, Dissolution and dispersion of coal in ionic liquids, *Energy Fuels*, 24 (2010) 1848-1853.
- 77 P. Painter, R. Cetiner, N. Pulati, M. Sobkowiak, J.P. Mathews, The dispersion of liquefaction catalysts in coal in ionic liquids, *Energy Fuels*, 24 (2010) 3086-3092.
- 78 J.P. Mathews, V. Ferdandez-Alos, D.A. Jones, H.H. Schobert, Determining the molecular weight distribution of Pocahontas No. 3 low-volatile bituminous coal utilizing HRTEM and laser desorption ionization mass spectra data, *Fuel*, 89 (2010) 1461-1469.
- 79 T.J. Tambach, J.P. Mathews, F. van Bergen, Molecular exchange of CH<sub>4</sub> and CO<sub>2</sub> in coal: enhanced coalbed methane on a nanoscale, *Energy Fuels*, 23 (2009) 4845-4847.
- 80 N. Sarunac, M. Ness, C. Bullinger, J.P. Mathews, P. Halleck, A novel fluidized bed drying and density segregation process for upgrading low-rank coals, *International Journal of Coal Preparation and Utilization*, 29 (2009) 317-332.
- 81 J.D.N. Pone, M. Hile, P.M. Halleck, J.P. Mathews, Three-dimensional carbon dioxide-induced strain distribution within a confined bituminous coal, *International Journal of Coal Geology*, 77 (2009) 103-108.
- 82 J.D.N. Pone, P.M. Halleck, J.P. Mathews, Sorption capacity and sorption kinetic measurements of CO<sub>2</sub> and CH<sub>4</sub> in confined and unconfined bituminous coal, *Energy Fuels*, 23 (2009) 4688-4695.

- 83 M.R. Narkiewicz, J.P. Mathews, Visual representations of carbon dioxide adsorption in a low-volatile bituminous coal molecular model, *Energy Fuels*, 23 (2009) 5326-5246.
- 84 Y.-C. Hsu, Y.-H. Ching, J.P. Mathews, A. Carr-Chellman, Undergraduate students' self-regulated learning experience in a web-based learning environment, *Quarterly Review of Distance Education*, 10 (2009) 109-121.
- 85 D. Van Niekerk, R.J. Pugmire, M.S. Solum, P. Painter, J.P. Mathews, Structural characterization of vitrinite-rich and interinite-rich Permian aged South African coals, *International Journal of Coal Geology*, 76 (2008) 290-300.
- 86 M.R. Narkiewicz, J.P. Mathews, Improved low-volatile bituminous coal representation: incorporating the molecular weight distribution, *Energy Fuels*, 22 (2008) 3104-3111.
- 87 J.P. Mathews, S. Eser, P.G. Hatcher, A.W. Scaroni, The shape of pulverized bituminous vitrinite coal particles, *KONA Powder and Particle*, 25 (2007) 145-152.
- 88 P.C. Painter, M. Sobkowiak, J.P. Mathews, A. Scaroni, Concerning the nature of coal solutions and suspensions, *Energy Fuels*, 18 (2004) 1104-1107.
- 89 H. Groenzin, O.C. Mullins, S. Eser, J.P. Mathews, M.G. Yang, A.D. Jones, Molecular size of asphaltene solubility fractions, *Energy Fuels*, 17 (2003) 498-503.
- 90 J.P. Mathews, P.G. Hatcher, A.W. Scaroni, Proposed model structures for Upper Freeport and Lewiston-Stockton vitrinites, *Energy Fuels*, 15 (2001) 863-873.
- 91 M. Acharya, M.S. Strano, J.P. Mathews, J.L. Billinge, V. Petkov, S. Subramoney, H.C. Foley, Simulation of nanoporous carbons: a chemically constrained structure, *Philosophical Magazine B-Physics of Condensed Matter Statistical Mechanics Electronic Optical and Magnetic Properties*, 79 (1999) 1499-1518.
- 92 J.P. Mathews, P.G. Hatcher, A.W. Scaroni, Particle size dependency of volatile matter: Is there a non-maceral related effect?, *Fuel*, 76 (1997) 359-362.
- 93 J.-L. Faulon, J.P. Mathews, G.A. Carlson, P.G. Hatcher, Correlation between micropore and fractal dimension of bituminous coal based on computer generated models, *Energy Fuels*, 8 (1994) 408-415.

#### *Book Chapters*

- 1 J. Rempel, J. Halverson, C. Burket, M.S. Strano, J.P. Mathews, H.C. Foley, Structural Modeling of Nanoporous Carbon: A Review of Approaches to Simulating an Aperiodic and Non-Equilibrium Solid, in: M.W. Thorpe, S.J. Billinge (Eds.) *From Semiconductors to Proteins: Beyond the Average Structure*, a Volume in the *Fundamental Materials Research Series*, Kluwer, New York, 2001.
- 2 P.G. Hatcher, J.-L. Faulon, D.J. Clifford, J.P. Mathews, A Three-dimensional Structural model for Humic Acids from Oxidized soil, in: N. Senesi, T.M. Miano (Eds.) *Humic Substances in the Global Environment and Implications on Human Health*, Elsevier Science B. V., 1994, pp. 133-138.

#### *Conference Papers (technical, not peer reviewed)*

- 1 Q. Chang, W. Zhu, J.K. Watson, F. Wang, J.P. Mathews, An image-guided rapid soot structure construction strategy, in: *The World Conference on Carbon*, Lexington, KY, 2019, pp. 1-3.

- 2 C. Wang, H. Xin, J.K. Watson, J.P. Mathews, Comparison of char reactivity and  
behavior between oxy-fuel and air combustion using a simplified atomistic  
simulation, in: 37th International Symposium on Combustion, 2018.
- 3 W. Zhu, C. Wang, R. Vander Wal, J.P. Mathews, A 2D fingerprinting approach for  
structural visualization of complex 3D soot atomistic representations, in: The World  
Conference on Carbon, State College, PA, 2016, pp. 1-3.
- 4 H. Xin, C.-H. Huang, J.P. Mathews, An exploration of char reactivity capturing  
temperature effects within a simplistic but large-scale atomistic simulation, in: The  
World Conference on Carbon, State College, PA, 2016, pp. 1-3.
- 5 C. Wang, H. T., C.-H. Huang, R.L. Vander Wal, E. Lester, J.P. Mathews, Improved  
curvature analysis for HRTEM lattice fringes applied to soot, in: The World  
Conference on Carbon, State College, PA, 2016, pp. 1-4.
- 6 B. Thanasattayaviboon, J.P. Mathews, Porosity and morphology transformations of  
Pittsburgh no. 8 coal char in CO<sub>2</sub> gasification under pore diffusion limitation, in:  
The World Conference on Carbon, State College, PA, 2016, pp. 1-4.
- 7 Y. Huang, F.S. Cannon, J. Gao, J.K. Watson, J.P. Mathews, Atomistic modeling insight  
into the structure of lignite-based activated carbon, and behavior of benzene  
sorption, in: The World Conference on Carbon, State College, PA, 2016.
- 8 H.H. Xin, C. Wang, D. Wang, J.P. Mathews, Examination of changing char reactivity  
with isothermal oxy-fuel combustion by a simplified atomistic simulation, in:  
International Pittsburgh Coal Conference, Pittsburgh, USA, 2015, pp. 1-7.
- 9 H.H. Xin, C. Wang, D. Wang, J.P. Mathews, Simplified atomistic simulation of coal char  
oxy-combustion: sensitivity analysis for reaction distance and factors influencing  
oxygen penetration, in: International Conference on Coal Science and Technology,  
Melbourne, Australia, 2015, pp. 1-4.
- 10 H. Xin, C. Wang, E. Louw, J.K. Watson, J.P. Mathews, Coal char atomistic exploration  
of oxy-combustion reactivity, in: 8th International Conference on Coal Combustion,  
Beijing, China, 2015, pp. 1-3.
- 11 J.P. Mathews, T. Huddle, C. Wang, E. Lester, Quantifying curvature in coal HRTEM  
lattice fringe micrographs, in: International Conference on Coal Science and  
Technology, Melbourne, Australia, 2015.
- 12 J.P. Mathews, Plenary Lecture and paper: The structure and behavior of coals and  
chars via atomistic simulations of pyrolysis and combustion, in: 8th International  
Conference on Coal Combustion, Beijing, China, 2015, pp. 1-5.
- 13 R.E. Winans, S. Seifert, M.J. Calo, J.P. Mathews, K. Gilbert, J. Wang, D. Lock,  
Characterization of coal porosity and gas-solid interfaces by SAXS, in: International  
Conference on Coal Science & Technology, The Pennsylvania State University, PA,  
USA, 2013, pp. 889-895.
- 14 M.J. Roberts, R.C. Everson, H.W.J.P. Neomagus, C.G.C.E. Van Sitter, D. Van Niekerk, J.P.  
Mathews, The molecular structure of selected South African coal-chars to elucidate  
fundamental principles of the reaction between char and carbon dioxide, in:  
International Conference on Coal Science & Technology, The Pennsylvania State  
University, PA, USA, 2013, pp. 91-103.
- 15 V. Ramachandran, F. Castro-Marcano, D. Van Niekerk, V. Ferdandez-Alos, Y.E.  
Alvares Rojas, J.O. Pou, J.K. Watson, J.P. Mathews, Construction, structural  
evaluation, and exploring chemical transformations of coal molecular models using

- scripting, in: International Conference on Coal Science & Technology, The Pennsylvania State University, PA, USA, 2013, pp. 1015-1026.
- 16 G.D. Mitchell, J.P. Mathews, Penn State's Coal Repository: Penn State and Argonne Premium Coal Sample Bank & Database, in: International Conference on Coal Science & Technology, The Pennsylvania State University, PA, USA, 2013, pp. 1122-1132.
- 17 J.P. Mathews, V. Ramachandran, F. Castro-Marcano, A.C.T. Van Duin, K.B. Anderson, Exploring oxidative hydrolysis dissolution (OHD) reaction chemistry of Illinois no. 6 coal with molecular modeling approaches, in: Clearwater Clean Coal Conference, Clearwater, FL, 2013, pp. 936-945.
- 18 E. Louw, J.K. Watson, J.P. Mathews, Evaluating combustion reactivity of large-scale molecular coal char models with control over structural features, in: International Conference on Coal Science & Technology, The Pennsylvania State University, PA, USA, 2013, pp. 569-576.
- 19 E. Louw, J.K. Watson, J.P. Mathews, An alternate construction approach for large-scale atomistic representations of carbon with controls over structural diversity and orientation, in: Annual World Conference on Carbon, Rio De Janeiro, Brazil, 2013, pp. 1-2.
- 20 H. Kumar, D. Elsworth, J.P. Mathews, Evaluation of the role of coal softening on permeability for a sand propped fracture, in: International Conference on Coal Science & Technology, The Pennsylvania State University, PA, USA, 2013, pp. 1485-1491.
- 21 Q.P. Campbell, J. Viljoen, M. le Roux, J.P. Mathews, Following coal processes using micro focus X-ray computed tomography, in: International Conference on Coal Science & Technology, The Pennsylvania State University, PA, USA, 2013, pp. 881-888.
- 22 J.P. Mathews, R.E. Winans, R. Rodgers, A. Sharma, Advances in coal analysis and simulation 1989-2012, in: International Pittsburgh Coal Conference, Pittsburgh, PA, USA, 2012, pp. 1-11.
- 23 J.P. Mathews, C. Song, B. Finkelman R., W. Yue, Chinese coal-in-title journal articles in Chinese and English, in: International Pittsburgh Coal Conference, Pittsburgh, PA, USA, 2012, pp. 1-15.
- 24 H. Kumar, D. Elsworth, J.P. Mathews, J. Liu, D. Pone, The dynamic permeability of propped and non-propped artificial fracture in granite and bituminous coal with changes in effective stress, in: International Pittsburgh Coal Conference, Pittsburgh, PA, USA, 2012, pp. 1-9.
- 25 F. Castro-Marcano, A.C.T. van Duin, J.P. Mathews, ReaxFF molecular dynamics pyrolysis simulation of a large-scale molecular model of Illinois no. 6 coal including the role of organic sulfur, in: International Pittsburgh Coal Conference, Pittsburgh, PA, USA, 2012.
- 26 R.E. Winans, S. Seifert, D. Locke, P. Chupas, K. Chapman, M.R. Narkiewicz, J.P. Mathews, J. Calo, Porosity and gas absorption of coals studied by X-ray scattering and modeling, in: International Conference on Coal Science & Technology, Oviedo, Spain, 2011, pp. 1-8.

- 27 S. Wang, H. Kumar, G. Izadi, J. Liu, D.-S. Lee, J.P. Mathews, D. Pone, D. Elsworth, Permeability evolution in naturally-fractured sorbing media: coals and tight shales, in: GeoProc2011, Perth, Australia, 2011.
- 28 J.P. Mathews, B.G. Miller, C.S. Song, H.H. Schobert, F. Botha, R.B. Finkelman, A. Chaffee, The current state of affairs of coal research in the United Kingdom, Germany, Australia, and South Africa, in: International Conference on Coal Science and Technology, Oviedo, Spain, 2011.
- 29 J.P. Mathews, B. Miller, C.S. Song, H.H. Schobert, F. Botha, R.B. Finkelman, The current state of affairs of coal research in U.S. Universities, in: International Conference on Coal Science and Technology, Oviedo, Spain, 2011.
- 30 J.P. Mathews, V. Krishnamoorthy, E. Louw, A.H.N. Tchapda, F. Castro-Marcano, V. Karri, D.A. Alexis, G.D. Mitchell, Coal, it is elementary my dear Watson, in: International Pittsburgh Coal Conference, Pittsburgh, PA, 2011.
- 31 J.P. Mathews, F. Castro-Marcano, V. Ferdandez-Alos, J.K. Watson, Y.E. Alvarez, D. Van Niekerk, A.M. Kamat, M.F. Russo, A. van Duin, Breaking the barriers: accurate large-scale molecular representations of coal (or other carbonaceous structures) with relative ease and their use with reactive simulations, in: Prepr. Pap.-Am. Chem. Soc., Div. Fuel Chem., Denver, CO, 2011, pp. 295-297.
- 32 J.P. Mathews, Y.E. Alvarez, R.E. Winans, An analysis of the research performed with the Argonne Premium Coals and its contribution to coal science, in: International Conference on Coal Science & Technology, Oviedo, Spain, 2011, pp. 1-8.
- 33 E. Louw, G.D. Mitchell, J.P. Mathews, Morphologies, X-ray parameters, and burnout comparisons of inertinite-rich and vitrinite-rich South African bituminous coal derived chars, in: International Pittsburgh Coal Conference, Pittsburgh, PA, 2011.
- 34 H. Kumar, D. Elsworth, J.P. Mathews, S. Wang, J. Liu, D. Pone, Optimization of CO<sub>2</sub>-enhanced coalbed methane recovery accomodating swelling-induced permeability evolution, in: American Rock Mechanics Association, Beijing, China, 2011.
- 35 H. Kumar, D. Elsworth, D.S. Lee, J.P. Mathews, C. Marone, Evolution of shale and coal permeability under differential sorption of He, CH<sub>4</sub> and CO<sub>2</sub>, in: ARMA, 2011.
- 36 D. Elsworth, S. Wang, G. Izadi, H. Kumar, J. Liu, D.-S. Lee, J.P. Mathews, D. Pone, Complex process couplings in systems pushed far from equilibrium: applications to carbon dioxide sequestration in carboniferous formations [Plenary], in: Proc. Workshop on CO<sub>2</sub> Storage in Carboniferous Formations and Abandoned Mines, China University of Mining and Technology, Beijing, 2011, pp.?
- 37 F. Castro-Marcano, R.E. Winans, S. Seifert, D. Locke, P. Chupas, K. Chapman, J.M. Calo, J.P. Mathews, Fine structure evaluation of the pair correlation function with molecular "slice" models of the Argonne Premium coals, in: International Pittsburgh Coal Conference, Pittsburgh, PA, 2011.
- 38 F. Castro-Marcano, A.M. Kamat, M.F. Russo, A. van Duin, J.P. Mathews, ReaxFF molecular dynamics oxidation simulation of Illiinois No. 6 coal char in: Prepr. Pap.-Am. Chem. Soc., Div. Fuel Chem., Denver, CO, 2011, pp. 276-278.
- 39 Y.E. Alvarez, J.C.K. Watson, J.O. Pou, F. Castro-Marcano, J.P. Mathews, Visualizing the macromolecular network structure of a large-scale (50,000 atom) Illinois No. 6 coal bituminous molecular representation in 3D and 2D lattice views, in: International Conference on Coal Science & Technology, Oviedo, Spain, 2011.

- 40 Y.E. Alvarez, B.M. Moreno, M.T. Klein, J.K. Watson, J.P. Mathews, Network decomposition modeling in coal-specific lattices, in: Prepr. Pap.-Am. Chem. Soc., Div. Fuel Chem., Denver, CO, 2011, pp. 285-287.
- 41 P. Painter, N. Pulati, R. Cetiner, M. Sobkowiak, G.D. Mitchell, J.P. Mathews, Dissolution and dispersion of coal in ionic liquids, in: Prepr. Pap.-Am. Chem. Soc., Div. Fuel Chem., 2010, pp. 19-20.
- 42 H. Kumar, D. Elsworth, J.P. Mathews, C. Marone, Evolution of shale and coal permeability under differential sorption of He, CH<sub>4</sub>, and CO<sub>2</sub>, in: AGU Conference, 2010.
- 43 Y.E. Alvarez, J.K.W. Watson, J.P. Mathews, Improving the utility of large-scale coal molecular models by simplifying the view: 3D models to reactive lattice grids, in: Prepr. Pap.-Am. Chem. Soc. Div. Fuel Chem., Boston, MA, Aug. 22-26, 2010, pp. 382-383.
- 44 D. Van Niekerk, J.P. Mathews, Molecular dynamics simulation of coal-solvent interactions in Permian-aged South African coals, in: International Conference on Coal Science & Technology, Cape Town, South Africa, 2009.
- 45 J.P. Mathews, A. van Duin, A. Chaffee, The utility of coal molecular models, in: International Conference on Coal Science & Technology, Cape Town, South Africa, 2009.
- 46 J.P. Mathews, J.D.N. Pone, G.D. Mitchell, P. Halleck, High-resolution X-ray computed tomography observations of the thermal drying of lump-sized subbituminous coal, in: International Conference on Coal Science & Technology, October 26-29, Cape Town, South Africa, 2009.
- 47 V. Fernandez-Alos, J.K. Watson, J.P. Mathews, Directly capturing aromatic structural features in coal via "Fringe3D" generating 3D molecular models directly from HRTEM lattice fringe images, in: Prepr. Pap.-Am. Chem. Soc., Div. Fuel Chem., Salt Lake City, UT, 2009, pp. 338-340.
- 48 R.E. Winans, K.W. Chapman, P.J. Chupas, S. Seifert, A.H. Clemens, J. Calo, E. Bain, J.P. Mathews, M.R. Narkiewicz, In situ studies of coal pressurized with CO<sub>2</sub> by small angle and high energy, wide angle X-ray scattering, in: Prepr. Pap. - Am. Chem. Soc., Div. Fuel Chem., New Orleans, LA, 2008, pp. 283-285.
- 49 J.D.N. Pone, P.M. Halleck, J.P. Mathews, Methane and carbon dioxide sorption and transport rates in coal at in-situ conditions, in: 9th International Conference on Greenhouse Gas Control Technologies, Washington, D.C., 16-20 November, 2008.
- 50 J.D.N. Pone, P.M. Halleck, J.P. Mathews, Detailed characterization of coal strains induced by compression, carbon dioxide sorption, and desorption at simulated in situ conditions-conf paper, in: 2008 Asia Pacific Coalbed Methane Symposium, Brisbane, Australia, 22-24 September, 2008.
- 51 D. Van Niekerk, J.P. Mathews, The nature of solvent extracts from vitrinite-rich and inertinite-rich South African bituminous coals, in: International Pittsburgh Coal Conference, Sandton, South Africa, 2007.
- 52 D. Van Niekerk, J.P. Mathews, Solvent swelling of similar rank South African vitrinite-rich and inertinite-rich coals: swelling extent and maceral influences, in: International Conference on Coal Science and Technology, The University of Nottingham, England, 28-31 August, 2007.

- 53 J.P. Mathews, G.D. Cody, A. Sharma, The structural alignment of coal as measured by image analysis of HRTEM fringes, in: International Conference on Coal Science and Technology, The University of Nottingham, England, 28-31 August, 2007.
- 54 S. Kingman, E. Lester, T. Wu, J.P. Mathews, S. Bradshaw, The potential of coal microwaving in power stations to improve grindability, in: International Conference on Coal Science and Technology, The University of Nottingham, England, 28-31 August, 2007, pp. 1-13.
- 55 D. van Niekerk, B. Markley, Y. Li, V. Rodriguez-Santiago, D. Thompson, A.R. Mohan, D. Elsworth, J.P. Mathews, S. Pisupati, C. Song, Utilization of carbon dioxide from coal-fired power plant for the production of value-added products, in: The International Pittsburgh Coal Conference, Pittsburgh, PA, September 25-28, 2006.
- 56 N. Soundarrajan, M.A. Hill, L.-M. Chen, V.G. Dhar, J. Guo, H.J. Kim, O. Mustafaoglu, R. Sundararaman, D. Elsworth, J.P. Mathews, S.V. Pisupati, C. Song, Optimal design for integrating CO<sub>2</sub> capture and fuel conversion technologies in a 500 MWe coal-based power plant, in: The International Pittsburgh Coal Conference, Pittsburgh, PA, September 25-28, 2006.
- 57 M.R. Narkiewicz, J.P. Mathews, Visualization of carbon dioxide sequestration issues within coal using a molecular representation of Pocahontas No. 3 coal, in: 12th International Conference on Coal Science and Technology, October 9-14, Okinawa, Japan, 2005.
- 58 T.J. Dick, O. Acevedo, P. Dalal, J.D. Madura, J.D. Evanseck, J.P. Mathews, Molecular basis for carbon dioxide sequestration in coal, in: Prepr. Pap. - Am. Chem. Soc., Div. Fuel Chem., Orlando, FL, April 7-11, 2002, pp. 14-16.
- 59 A.N. Adams, J.P. Mathews, H.H. Schobert, The use of image analysis for the optimization of pre-baked anode formulation, in: Light Metals: Proceedings of Sessions, TMS Annual Meeting, Warrendale, Pennsylvania, 2002, pp. 547-552.
- 60 A.N. Adams, C.O. Karacan, A. Grader, J.P. Mathews, P. Halleck, H.H. Schobert, The non-destructive 3-D characterization of pre-baked carbon anodes using X-ray computerized tomography, in: Light Metals: Proceedings of Sessions, TMS Annual Meeting, Warrendale, Pennsylvania, 2002, pp. 535-539.
- 61 J.P. Mathews, O. Karacan, P. Halleck, G.D. Mitchell, A. Grader, Storage of pressurized carbon dioxide in coal observed using X-ray tomography, in: First National Conference on Carbon Sequestration, Washington, DC, 2001.
- 62 J.P. Mathews, C.O. Karacan, R.P. Dutta, S. Eser, Computer tomography of laboratory generated delayed coke, in: Prepr. Pap. - Am. Chem. Soc., Div. Petro. Chem., Chicago, IL, 2001, pp. 252-255.
- 63 J.P. Mathews, A.D. Jones, P.J. Pappano, R. Hurt, H.H. Schobert, New insights into coal structure from the combination of HRTEM and laser desorption ionization mass spectrometry, in: 11th Int. Conf. on Coal Science, San Francisco, CA., 2001.
- 64 J.M. Andrésen, J.J. Strohm, J.P. Mathews, C. Song, Modeling of coke formation from naphthenic jet fuel in the pyrolytic regime, in: Prepr. Pap. - Am. Chem. Soc., Div. Fuel Chem., Chicago, IL, 2001, pp. 365-366.
- 65 A.N. Adams, J.P. Mathews, H.H. Schobert, The use of image analysis for the optimization of pre-baked anode performance in aluminum production, in: Prepr. Pap. - Am. Chem. Soc., Div. Fuel Chem., Chicago, IL, 2001, pp. 595-596.

- 66 P.J. Pappano, J.P. Mathews, H.H. Schobert, Graphitization studies of Pennsylvania anthracite using molecular visualization, in: Eurocarbon 2000, 9-13 July, Berlin, 2000, pp. 165-166.
- 67 P.J. Pappano, J.P. Mathews, H.H. Schobert, Molecular modeling of the stages of carbonization of phenanthrene and anthracene, in: 24th Biennial Conference on Carbon, Charleston, SC, 1999, pp. 202-204.
- 68 P. Pappano, J.P. Mathews, H.H. Schobert, Structural determinations of Pennsylvania anthracites, in: Prepr. Pap. - Am. Chem. Soc., Div. Fuel Chem., New Orleans, 1999, pp. 567-570.
- 69 J.P. Mathews, S. Eser, P. Rahimi, Preliminary results on the molecular structures of the Athabasca and Cold Lake asphaltenes, in: Prepr. Pap. - Am. Chem. Soc., Div. Fuel Chem., New Orleans, 1999, pp. 783-785.
- 70 H.H. Schobert, F.J. Rusinko, J.P. Mathews, W(h)ither the coal industry? The long term view, in: The Pittsburgh Coal Conference, 1998.
- 71 J.P. Mathews, P.G. Hatcher, A.W. Scaroni, Devolatilization, a molecular modeling approach, in: Prepr. Pap. - Am. Chem. Soc., Div. Fuel Chem., Dallas, TX, March 29-April 2, 1998, pp. 136-140.
- 72 J.P. Mathews, P.G. Hatcher, S. Eser, P. Walsh, A.W. Scaroni, Time-temperature histories of bituminous coal particles in a drop-tube reactor, in: Prepr. Pap.-Am. Chem. Soc., Div. Fuel Chem., Boston, MA, August 22-27, 1998, 1998, pp. 611-615.
- 73 J.P. Mathews, P.G. Hatcher, A.W. Scaroni, Influence of chemical structure on the fluidity of rapidly heated bituminous vitrinites, in: Prepr. Pap. - Am. Chem. Soc., Div. Fuel Chem., San Francisco, April 13-17, 1997, pp. 214-217.
- 74 D.J. Clifford, J.P. Mathews, J.-L. Faulon, P.G. Hatcher, Chemical structure of hand-picked coal macerals derived from specific plant precursors, in: Prepr. Pap. - Am. Chem. Soc., Div. Fuel Chem., San Diego, 1994, pp. 198-204.
- 75 J.P. Mathews, A.W. Scaroni, J.-L. Faulon, P.G. Hatcher, A structural model for coalified wood (vitrinite) from a medium volatile bituminous coal seam, in: K.H. Michaelian (Ed.) Int. Conf. on Coal Science, Banff, Alberta, Canada, Int. Energy Agency, 1993, pp. 128-131.
- 76 J.-L. Faulon, J.P. Mathews, G.A. Carlson, P.G. Hatcher, Statistical evaluation of physical properties for coal macromolecules based on computer generated structures, in: Prepr. Pap. - Am. Chem. Soc., Div. Fuel Chem., Chicago, IL, 1993, pp. 1275-1280.

*Conference Papers Education Research*

- 1 S. Pisupati, J.P. Mathews, Differences in teaching and learning outcomes in face-to-face, online, and hybrid modes of energy conservation course, in: American Society for Engineering Education Annual Conference, Pittsburgh, PA, 2008.
- 2 J.P. Mathews, M. Wherley, E. Spielvogel, Reaching the masses, web enabled redesign of "Energy & the Environment" general education class, in: Prepr. Pap.-Am. Chem. Soc., Div. Pet. Chem., New Orleans, LA, 2008.
- 3 S. Eser, J.P. Mathews, J.C. Bridger, Integrating general education courses in natural science and social science using a common thread, for example Pennsylvania coal, in: Prepr. Pap.-Am. Chem. Soc., Div. Pet. Chem., New Orleans, LA, 2008.

- 4 J.P. Mathews, D. DiBiase, Institutional Perspective on Online Education at Penn State, in: P.R. Howell (Ed.) International Conference on Education and Information Systems, Technologies and applications: EISTA '06, Orlando, FL, 2006, pp. 29-32.
- 5 P.R. Howell, J.P. Mathews, S. Pisupati, D. Babb, R.H. Locklin, Designing on-line general education, natural science courses, in the College of Earth and Mineral Sciences (EMS), at the Pennsylvania State University, in: The 4th International Conference on Education and Information Systems, Technologies and Applications: EISTA '06, Orlando, Florida, July 20-23, 2006, pp. 12-17.
- 6 D.R. Morales, J.P. Mathews, Success in online learning: Does faculty intercession via e-mail message alter student procrastination behavior and enhance learning?, in: *American Society for Engineering Education Annual Conference*, June 12-15, Portland, OR, 2005.
- 7 J.P. Mathews, A. Wiesner, S.V. Pisupati, What online quizzing can tell us about our students, in: *American Society for Engineering Education Annual Conference*, June 12-15, Portland, OR, 2005.
- 8 S. Pisupati, J.P. Mathews, D. DiBiase, A.W. Scaroni, An assessment of active and project based learning in energy conservation education for non-technical students, in: *Proceedings of the 2004 ASEE Annual Conference & Exposition*, 2004.
- 9 J.P. Mathews, N.A. Haughton, D. DiBiase, S. Pisupati, For an online course encompassing "traditional students": How, where, and when students work and engage with the course material, in: *Frontiers in Education Conference*, Savannah, Georgia, 2004, pp. 1-5.
- 10 S. Pisupati, J.P. Mathews, A.W. Scaroni, Energy conservation education for non-engineering students and effectiveness of active learning components, in: *American Society for Engineering Education Annual Conference*, Nashville, TN, 2003.
- 11 J.P. Mathews, E. Spielvogel, M. Wherley, D. DiBiase, S. Pisupati, Online teaching of "Energy & the Environment", in: *American Society for Engineering Education Annual Conference*, Nashville, TN, 2003.

*Ph.D Thesis Supervised*

1. Kumar, H. Poromechanical response of naturally fractured sorbing media. Ph.D. thesis, The Pennsylvania State University, 2014.\*
2. Louw, E. Structure and combustion reactivity of inertinite-rich and vitrinite-rich South African coal chars: quantification of the structural factors contributing to reactivity differences. Ph.D., The Pennsylvania State University, 2013.
3. Castro-Marcano, F. Improved generation of large-scale atomistic representations and pyrolysis/combustion simulations of Illinois coal and char using the ReaxFF reactive force field. The Pennsylvania State University, 2012.
4. Pone, J. D. N. Carbon dioxide sequestration in coal: characterization of matrix deformation, sorption capacity and dynamic permeability at in-situ stress conditions. Ph.D., The Pennsylvania State University, 2009.\*
5. Van Niekerk, D. Structural elucidation, molecular representation and solvent interactions of vitrinite-rich and inertinite-rich South African coals. The Pennsylvania State University, 2008.

\* co-advised student

### *MS Thesis Supervised*

- 1 C. Otis, Reforestation and afforestation may aid high density, low emission energy production In reducing CO2 and slowing climate change, in, Masters of Geographic Information Systems, The Pennsylvania State University, 2022.
- 2 D. Sagzhanov, 3D discrete fracture network for cleat-scale modeling of dynamic coal behavior, in: Energy and Mineral Engineering (Mining option), The Pennsylvania State University, 2019.
- 3 B. Thanasattayaviboon, Porosity, morphology, and structural transformation of bituminous coal char conversion under pore diffusion limitation: A comparison of CO2 gasification conversion and burnout in oxy-fuel combustion, in: Energy and Mineral Engineering, The Pennsylvania State University, 2016.
- 4 H. Kumar, Poromechanical response of naturally fractured sorbing media, in: Energy & Mineral Engineering, The Pennsylvania State University, 2014.
- 5 S. Pool, A preliminary natural gas resource assessment of the Marcellus Shale for West Virginia using basic geologic data and GIS, in: Geography, The Pennsylvania State University, 2013, pp. 1-67.
- 6 E. Louw, Structure and combustion reactivity of inertinite-rich and vitrinite-rich South African coal chars: quantification of the structural factors contributing to reactivity differences, in: Energy and Mineral Engineering, The Pennsylvania State University, 2013, pp. 1-212.
- 7 F. Castro-Marcano, Improved generation of large-scale atomistic representations and pyrolysis/combustion simulations of Illinois coal and char using the ReaxFF reactive force field, in: John and Willie Leone Family Department of Energy and Mineral Engineering, The Pennsylvania State University, 2012.
- 8 R. Cetiner, Fragmentation of coal and improved dispersion of liquefaction catalysts using ionic liquids, in: John and Willie Leone Family Department of Energy and Mineral Engineering, The Pennsylvania State University, 2011.
- 9 Y.E. Alvarez, Development of a reactive coarse-graining approach for the utility enhancement of complex large-scale molecular models of coal, in: Energy and Mineral Engineering, The Pennsylvania State University, State College, PA, 2011.
- 10 H. Kumar, Inducing fractures and cleat aperture enhancement in bituminous coal via the application of microwave energy applied under hydrostatic stress conditions, in: Energy & Mineral Engineering, The Pennsylvania State University, 2010.
- 11 V. Ferdandez-Alos, Improved molecular model generation from soots, chars, and coals: HRTEM lattice fringes reproduction with Fringe3D, in: Energy & Mineral Engineering, The Pennsylvania State University, 2010.
- 12 J.D.N. Pone, Carbon dioxide sequestration in coal: characterization of matrix deformation, sorption capacity and dynamic permeability at in-situ stress conditions, in: Energy & Mineral Engineering, The Pennsylvania State University, 2009.
- 13 D. Van Niekerk, Structural elucidation, molecular representation and solvent interactions of vitrinite-rich and inertinite-rich South African coals, in: Energy & Mineral Engineering, The Pennsylvania State University, 2008.

### **Awards**

Faculty Advising Award, College of Earth and Mineral Sciences, 2022

American Chemical Society Fellow, inducted 2016  
Outstanding Service, Energy and Fuels Technical Division, American Chemical Society 2016  
Honorable mention for Best Paper Pittsburgh Coal Conf. 2012  
2011 Best Poster (supervising Enette Louw), and honorable mention Best Paper (supervising Fidel Castro-Marcano) International Pittsburgh Coal Conference, Pittsburgh  
EMS Energy Institute Research Productivity Award (2010)  
Wilson Award for Outstanding Teaching (2006)  
Best Papers within the ECCD symposium co-author (ASEE-2004)  
Best Overall use of ANGEL Prize (ANGEL DAY II – 2004)  
John A. Dutton e-Education Fellowship (2003, 2004, & 2006, 2007)  
Mitchell Award for Innovative Teaching (2001)  
Recipient 1999 award for Employee Dedication (Energy Institute)  
Recipient 1998 C. C. Wright Award, (Excellence in Graduate Studies)  
Twice (1994 & 1996) the recipient of the annual Outstanding Service Award for the Energy & Fuels Research Center

### **Plenary, Keynotes, and Invited Presentations**

Mathews, J. P., **Invited Keynote:** Large-scale atomistic evaluations of coal char reactivity in oxygen: Following porosity and pore size development. In *IST International Workshop on Oxy-fuel Combustion*, Montabaur, Germany, 2015

Xin, H.; Wang, C.; Louw, E.; Watson, J. K.; Mathews, J. P. *Coal char atomistic exploration of oxy-combustion reactivity*, **Invited Plenary** at the 8th International Conference on Coal Combustion, Beijing, China, 2015; Beijing, China, 2015

Mathews, J. P., **Invited presentation:** Coal Structure and Behaviors a Mixture of Approaches. In *Pennsylvania Coal Ash Research Group*, Penn State, 2015

Mathews, J. P., **Invited presentation:** Meaningful Student Feedback". *eConversations*, Dutton Education Institute, the Pennsylvania State University 2014,

Mathews, J. P., **Invited presentation:** Quantifying, incorporating, and using structural diversity within coal". *Canadian Centre for Clean Coal/Carbon and Mineral Processing Technologies*, University of Alberta, Canada 2014

Mathews, J. P., **Invited presentation:** Coal structure molecular models and their utility. In *Thermochemical Conversion Workshop*, University of Delaware, 2013.

Mathews, J. P., **Invited presentation:** Advancing the creation of large-scale coal and coal-char atomistic representations. In *EMS Energy Institute Energy Exchange*, The Pennsylvania State University, PA, USA, 2013

Mathews, J. P., **Plenary:** One hundred things you did not know about coal. In *International Conference on Coal Science & Technology*, The Pennsylvania State University, PA, USA, 2013. (note self-invited when speaker was unable to attend).

Mathews, J. P., **Invited presentation:** The Walker Memorial: Coal research benefits from carbon science: repaying the favor with transferable coal/char molecular modeling advances In *Annual World Conference on Carbon*, Rio de Janeiro, Brazil, 2013

Tuana, N., (Moderator), Becker, C.; Maruszewski, S.; Mathews, J. P.; Monahan, R.; Moser, P.; Richard, T., **Roundtable discussion:** Penn State's Energy Future. *Berg Auditorium, Life Sciences, University Park*, 2009, Sponsored by Rock Ethics, Office of Physical Plant, and PSIEE.

Richards, T.; Santavavicca, D.; Mathews, J. P.; Grimes, C., **Briefing of Congressional Aids:** CO<sub>2</sub> can it fuel a nation? *Capital Building Complex, Longworth building, Washington D.C.* **2009.**

Mathews, J. P.; van Duin, A.; Chaffee, A., **Keynote:** The utility of coal molecular models. In *International Conference on Coal Science & Technology*, Cape Town, South Africa, 2009

Mathews, J. P., **Invited presentation:** Coal past and future. *Shennango Campus, Honors Society* **2009.**

Mathews, J. P., **Invited presentation:** Carbon dioxide sequestration in coal: molecular modeling and X-ray computed tomography observations. *Colorado School of Mines, Golden, CO* **2009.**

Mathews, J. P., **Presentation at Sponsor Meeting:** Microwave-induced fractures in coal. *Research Partnership for a Secure Energy for America, Golden, CO* **2009.**

Mathews, J. P., **Invited presentation:** 50 things you didn't know about coal. *Westmoreland Museum of American Art, Greensburg, PA* **2009.**

Mathews, J. P., **Invited presentation:** Application of high-resolution X-ray computed tomography to coal. *Coal Research Group, North-West University: Potchefstroom*, **2009.**

Mathews, J. P., **Invited presentation:** Coal molecular modeling, moving forward with large-scale modeling. *Gordon Conference on Hydrocarbon Resources* **2009**, Ventura, California.

Mathews, J. P., **Invited presentation:** The legacy of coal and its art. *Sponsored by EMS museum and Art Gallery and The Centre County Historical Society* **2009**, Match Factory Place, Bellefonte, PA

## **Past Funding**

Note departmental funding is also obtained via summer teaching. Sasol awards did not include tuition or student stipends that were paid directly from Sasol.

## **Reviewer**

Energy & Fuels, Fuel, International Journal of Coal Geology, Fuel Processing Technology, Journal of Applied and Analytical Pyrolysis, Carbon, Chemical Engineering Science, Molecular Physics, and others. Currently review ~25 articles per year.

## **Professional Societies and Service Positions**

Member of the Guest Editor team for two special issues of Fuel

Advisory Board Energy & Fuels, American Chemical Society journal, (2016-2022)

Chair 2013 International Conference on Coal Science and Technology (held at the Penn State Conference Center)

The U.S. representative on the International Organizing Committee of the International Coal Science and Technology Conference (2011-current)

Chair Division of Energy and Fuels, 2012 American Chemical Society

Chair for Fuel Chemistry, 2012 American Chemical Society

Member of the Divisions of Petroleum, Chemical Education, & Fuel Chemistry (Petroleum and Fuel is now merged into the division of Energy and Fuels) American Chemical Society

Membership for Fuel Chemistry, Pre-print Subscriptions 2011 American Chemical Society

Member of the American Society of Engineering Educators

External Reviewer for Engineering Evaluation, University of the North West, South Africa 2012

External thesis reviewer for Universities in South Africa (multiple) and Australia (several).

## **University Service**

Faculty Senate (2018-2022)

Conflict of Interest Committee member (2016-2021)

Penn State Representative to the Coal Utilization Research Council (2015-current)

Graduate Fellowships and Awards Committee (2014-2017)

## **College Service**

Member Ad-Hoc Committee on the Status of Female Faculty (2016)

Member Associate Dean Search Committee (2016)

Chair of the EMS Museum Advising Committee (2008-2012)

Secretary EMS Museum Advising Committee (2005-2008)

Chair of the Fixed-Term & Research Advisory Committee (2007-2008)

Member (2006-2007)

AESEDA Strategic Planning Committee. (2008)

EMS Energy & EESI Institutes Promotion Committee. (2009-2012) as the tenure-line member

College Computing Committee (2004)

Co-chair Coal Research Thrust for the EMS Energy Institute

## **Department Service**

Faculty Activity Review Committee (2022)

Energy Engineering Undergraduate Program Chair (2018-2020)  
Interim Graduate Program Officer Energy and Geo-Environmental Engineering (2007-2008).  
Chair Fuel Science Awards  
Organizer Given Lecture Series  
Lead ABET Assessment for Energy Engineering (2016-2021)

### **Courses Taught**

EGEE 411W\* Energy Science and Engineering Laboratory Course (writing intensive course)  
EM SC First Year Seminar

### **Past Courses**

EGEE 101 Energy & the Environment (online, hybrid, and face-to-face)  
FSc 410 Fuel Technology Lab  
FSc 401 Introduction to Fuel Technology  
ENNEC 484 Energy Economics\*  
EGEE 410 & 411 Social Legacy of Pennsylvania Coal & the Technological Legacy of Pennsylvania Coal\*  
EGEE 580 Design Engineering\*,  
EGEE 102 Energy Conservation\*,  
EGEE 597a Coal Structure & Behavior.  
EGEE 401 Energy in a Changing World  
EGEE Petrol Processing\*  
EGEE 431 Chemistry of Fuels\*  
EM SC 580 CAUSE (2003) Industrial Revolution to Industrial Ecology\*  
EM SC 580 CAUSE (2013) The Energy New Deal Down Under\*  
EM SC 580 CAUSE (2015) Sustainable Energy in Scandinavia: one Region, Many Choices\*  
EM SC 100s Earth and Mineral Sciences First-Year Seminar\* (regular semester and LEAP summer version: combined with Energy and the Environment).

\* Team-taught classes.

### **Short Courses to Industry and Academia**

These are typically ~5 lectures.

Geosciences University of China (several times)

Tata Steel, India, 2015

Tsinghua University, China, 2015

North West University, Potchefstroom Campus, South Africa, 2013

Sasol, South Africa 2005