James D. Kubicki
Department of Earth, Environmental & Resource Sciences
The University of Texas at El Paso
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Education:

Ph.D., Yale University, Geochemistry, 1984-89,
Thesis - "Structure and kinetics of silicate melts and glasses: Computer simulations, vibrational spectroscopy, and chemical diffusion experiments."
B.S., California State University at Fullerton, 1979-83, Major: Geology; Minors: Chemistry, Mathematics

Professional Experience:
Chair, Department of Earth, Environmental & Resource Sciences, UTEP, 2015 to 2024
Professor of Geochemistry, The Pennsylvania State University 2010-2015
Associate Professor of Geochemistry, The Pennsylvania State University 2004-2010
Assistant Professor of Geochemistry, The Pennsylvania State University 1998-2004
Senior Principal Engineer, Computer Sciences Corporation, 1997-1998
National Research Council Associate; Naval Command, Control, and Ocean Surveillance Center - Research, Development, Test, and Evaluation Division, 1994-1996
Schlumberger Postdoctoral Fellow; California Institute of Technology, 1991-93
Carnegie Institution of Washington Postdoctoral Fellow, Geophysical Laboratory, 1989-90

Teaching Experience:
University of Texas at El Paso, 2015-Present - Introduction to Environmental Science, Graduate Seminar
The Pennsylvania State University, 1998-2015
Physical Geology, Environment Earth, Geochemical Processes, Environmental Geology, Hydrogeology, Mineral Equilibria, Principles of Geochemistry, Geochemical Kinetics

Honors and Fellowships:
Fellow of the American Chemical Society, 2021
Clay Minerals Society Pioneer in Clay Science Award, 2020
U.S. DOE "Ten at Ten" Award in the Scientific Ideas category, 2019
Committee on Science – American Chemical Society, 2019
College of Earth & Mineral Sciences Wilson Research Award, 2015
College of Earth & Mineral Sciences Mentoring Award, 2008
Program Chair - ACS Division of Geochemistry, 2004-05
National Research Council Associate Award, NCCOSC, 1994
Schlumberger Fellowship, California Institute of Technology, 1991
Ford Prize in Mineralogy, Yale University, 1989
Graduated with Honors, California State University at Fullerton, 1983

Professional Societies:
American Chemical Society
Soil Science Society of America
Geological Society of America
Geochemical Society
American Geophysical Union

Leadership Activities

Participated in NASEM workshop on Building Capacity to Meet Current and Future Challenges and Needs Facing the U.S. Mineral Resources Workforce. 2024

Co-organized symposium on "Critical Materials: Perspective from the industry, government, and research communities" for the 2023 American Chemical Society national meeting.

Co-organized workshop on "Preparing students for careers, licensure, and industry" at the 2022 Earth Educators' Rendezvous.

AGU Heads & Chairs webinar on "Implementing curriculum updates in a geoscience/environmental science program: An example from the University of Texas at El Paso – 2021

Led department effort to implement UTEP EDGE program in the undergraduate curriculum

Attended geoscience undergraduate and graduate education summits at the University of Texas at Austin – 2016 and 2019

Grants Completed

Title: Molecular modeling of NOM interactions with cations, mineral surfaces and PAHs
Investigators: James D. Kubicki
Source: The Office of Naval Research
Total Award Amount: $331,000 Total Award Period Covered: 10/01/98 – 09/30/01

Title: Adsorption of cations on mineral-aqueous solution interfaces at elevated temperatures
Investigators: James D. Kubicki and Serguei Lvov
Source: National Science Foundation
Total Award Amount: $140,000 Total Award Period Covered: 07/01/00 – 06/30/02

Title: Molecular simulation of atmospheric reactions on the surface of soot particles
Investigator: James D. Kubicki
Source: Petroleum Research Fund
Total Award Amount: $25,000 Total Award Period Covered: 09/01/00 – 08/31/02

Title: Molecular level analysis of macromolecule-surface interactions in bacterial adhesion
Investigators: Bruce Logan, Jon Chorover, James D. Kubicki, Darell Velegol, & Meny Elimelech
Source: National Science Foundation
Total Award Amount: $2,916,392 Total Award Period Covered: 01/01/01 – 08/31/05

Title: Stony Brook-BNL collaboration to establish a Center for Environmental Molecular Sciences
Investigators: Reeder R. J., Schoonen M. A., Grey C. P., Parise J. B., Phillips B., Jacobsen C., Fisher N. S., Halada G., Strongin D., and Kubicki J. D.
Source: National Science Foundation
Total Award Amount: Approximately $6,000,000 - PSU $392,500
Total Award Period Covered: 09/01/02 – 08/31/07

Title: Nanoscale complexity at the oxide/water interface

Investigators: David J. Wesolowski, Donald A. Palmer, Pascale Bénézeth and Ariel A. Chialvo (Chemical and Analytical Sciences Division - Oak Ridge National Laboratory); William A. Hamilton and George D. Wignall (Solid State Division - ORNL); Liyuan Liang (Environmental Sciences Division - ORNL); Peter T. Cummings (Chemical Technology Division - ORNL/University of Tennessee, joint); Neil C. Sturchio, Paul Fenter and H. Henry Teng (Environmental Research Division - *Argonne National Laboratory*); Serguei N. Lvov (Director, Center for Electrochemical Studies - *Pennsylvania State University*) and James D. Kubicki (Department of Geosciences - PSU); Michael L. Machesky (Watershed Science Section - University of Illinois/Illinois State Water Survey), and Michael J. Bedzyk (*Northwestern University)*
Source: Department of Energy
Total Award Amount: $3,800,000 Total Award Period Covered: 09/01/00 – 08/31/08

Title: Experimental and Theoretical Investigations on Adsorption of Extracellular Compounds onto Mineral Surfaces
Investigators: James D. Kubicki
Source: Petroleum Research Fund
Total Award Amount: $80,000 Total Award Period Covered: 09/01/04 – 8/31/06
Location of Project: The Pennsylvania State University, University Park, PA
Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.75

Title: Center for Environmental Kinetic Analysis
Investigators: Brantley S. L., Burgos W., Dempsey B., Heaney P.J., and Kubicki J. D.
Source: NSF - CHE-0431328
Total Award Amount: $6,700,000 Total Award Period Covered: 09/01/04 – 8/31/09
Location of Project: The Pennsylvania State University, University Park, PA
Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 1.00

Title: USDA National Needs Fellowship for Nanoscale Science and Engineering in Forest Resources
Investigators: Brown N., Richard T., Catchmark J., Kubicki J.D.
Source: USDA
Total Award Amount: $229,500 Total Award Period Covered: 01/01/07 – 12/31/11
Location of Project: The Pennsylvania State University, University Park, PA
Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.00

Title: Quantum mechanical calculation of hydrogen isotope exchange thermodynamics and kinetics on petroleum model compounds
Investigators: Kubicki J.D. and Freeman K.H.
Source: Petroleum Research Fund
Total Award Amount: $90,000 Total Award Period Covered: 09/01/07 – 8/31/09
Location of Project: The Pennsylvania State University, University Park, PA
Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.50

Title: Structure and properties of disordered iron-oxyhydroxides
Investigators: Grey C.P., Reeder R.J., Parise J.B., Phillips B.L., Strongin D.R., Morgan D., Kubicki J.D.
Source: NSF - CHE-0958664
Total Award Amount: $375,000 Total Award Period Covered: 09/01/07 – 8/31/12
Location of Project: The Pennsylvania State University, University Park, PA
Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.50

Title: "ARRA: Center for Lignocellulose Structure and Formation"
Sponsor: U.S. Department of Energy (DE-SC0001090)
Period of Performance: 8/1/2009 - 7/31/2015
Total Budget Requested: $23,790,000

Role: Faculty
Location of Project: The Pennsylvania State University
Effort (person months): 0.50 Acad 0.25 Sumr

Title: Collaborative Research: Quantifying the Reactive Surface Area of Environmental Solids
Source of Support: National Science Foundation
Total Award Amount: $610,000 (PSU - Mueller & Kubicki)
Period of Performance: 09/15/2012 – 08/31/15
Location of Project: The Pennsylvania State University
Person-Months per Year Committed to the Project: Cal: 0.00 Acad: 0.75 Sumr: 0.25

Title: Modeling Quartz Dissolution
Source of Support: Battelle - Oak Ridge National Laboratory
Total Award Amount: $125,000
Period of Performance: 07/01/2013 - 07/31/2015
Location of Project: The Pennsylvania State University
Person-Months per Year Committed to the Project: Cal: 0.00 Acad: 0.75 Sumr: 0.25

Title: Center for Lignocellulose Structure and Formation (CLSF)
Source of Support: U.S. Department of Energy
Total Award Amount: $13,200,000 (Approximately $80,000 to Kubicki.)
Period of Performance: 08/01/2014 - 07/31/2019
Location of Project: The Pennsylvania State University
Person-Months per Year Committed to the Project: Cal: 0.00 Acad: 0.0 Sumr: 0.5

Title: Collaborative Research: Toward a unified model for FHY nanoparticles behavior in the environment: a multipronged investigation of surface structure and reactivity
Source of Support: Georgia State University (NSF Primary SP00011816-03)
Total Award Amount: $47,873
Period of Performance: 01/01/2015 - 12/31/2018
Location of Project: The Pennsylvania State University
Person-Months per Year Committed to the Project: Cal: 0.00 Acad: 0.36 Sumr: 0.12

Title: In situ synchrotron X-ray diffraction of Fe oxide transformations in aqueous solutions
Sponsor: National Science Foundation 5381-UTEP-NSF-2211
Period of Performance: 11/1/2015 - 10/31/2019
Total Budget Requested: $399,465
Role: Co-Investigator
Location of Project: The Pennsylvania State University, UTEP
Effort (person months): 0.75 Acad 0.25 Sumr

Title: "FWP ERKCC72: Atomic- to Pore-Scale Geochemical Processes"
Sponsor: Department of Energy
Period of Performance: 04/18/2016 - 03/31/2019
Total Budget Requested: $155,000
Role: Co-Investigator
Location of Project: UTEP
Effort (person months): 0.0 Acad 0.50 Sumr

Title: "Competitive Adsorption of Phosphate and Lignin onto FeOOH: Insights from Experiments and Density Functional Theory"
Sponsor: USDA 2018-67019-27801
Period of Performance: 01/01/2018 - 12/31/2020
Total Budget Requested: $499,968 ($180,000 UTEP)
Role: Co-Investigator

Location of Project: UTEP
Effort (person months): 0.00 Acad 0.50 Sumr

Title: Center for Lignocellulose Structure and Formation (CLSF)
Source of Support: U.S. Department of Energy DE-SC0001090
Total Award Amount: $13,400,000 ($80,000 to Kubicki.)
Period of Performance: 08/01/2018 - 07/31/2023
Location of Project: The Pennsylvania State University
Person-Months per Year Committed to the Project: Cal: 0.00 Acad: 0.0 Sumr: 0.5

Title: "The origins of molecules in diverse space and planetary environments and their intramolecular isotope signatures"
Name of PI on Proposal: Kate Freeman (Penn State)
Program Name/Point of Contact: Science Mission Directorate, Planetary Science; Point of Contact (phone): Mary A. Voytek, (202) 358-1577
Sponsor: NASA SPN01191
Period of Performance: 01/01/2018 – 12/31/2023
Award Amount: $552,540
Effort (person months): Cal: 0.00 Acad: 0.00 Sumr: 0.25

Current Support

Title: "The Permian Energy Technology and Resilience Alliance (PETRA): Expanding Resilience of Energy Communities through Technology and Social Research"
Name of PI on Proposal: Brian Korgel (UT-Austin)
Sponsor: NSF Engines Program
Period of Performance: 05/01/2023 – 04/30/2025
Award Amount: $1,000,000 ($50,000 to Kubicki)
Effort (person months): Cal: 0.00 Acad: 0.00 Sumr: 0.50

Title: "Advanced Multi-Physics Machine Learning for Subsurface Energy Systems Across Scales"
Name of PI on Proposal: Son-Young Yi (UTEP)
Sponsor: DOE Geothermal Earthshot Program
Period of Performance: 01/01/2024 – 12/31/2026
Award Amount: $5,248,752
Effort (person months): Cal: 0.00 Acad: 0.00 Sumr: 1.00

Title: "SRG – Developing Biomimetic Binding Sites in Metal-Organic Frameworks for the Separation of Critical Rare Earth Elements"
Name of PI on Proposal: James D. Kubicki (UTEP)
Sponsor: Sandia National Laboratories
Period of Performance: 10/01/2023 – 09/30/2024
Award Amount: $98,912
Effort (person months): Cal: 0.00 Acad: 0.00 Sumr: 0.00

Title: "Evaluating New Materials and Processes for Radioactive Tank Waste Processing: Workforce Development in *f*-Element Chemistry, Nuclear Chemical Engineering, and Supply Chain Management (NuChemE Pipeline)"
Name of PI on Proposal: Catherine Brewer (NMSU)
Sponsor: 2023 Department of Energy Office of Environmental Management (DOE-EM) Minority Serving Institutions Partnership Program (MSIPP)

Period of Performance: 01/01/2024 – 12/31/2026
Award Amount: $4,827,097
Effort (person months): Cal: 0.00 Acad: 0.00 Sumr: 1.00

Students Supervised:

Graduate Students

Jiye Guo, Amanda Labrado, Nathan Reade, The University of Texas at El Paso (Ph.D.)
Seyi Ajayi, Brendan Puls, The Pennsylvania State University (M.S.)
Jason Boettger, Mark DelloStritto, Christin Morrow, Kramer Campen, Kideok Kwon, Shawn Domagal-Goldman, Heath Watts, The Pennsylvania State University (Ph.D.)
Matthew Wander, SUNY Stony Brook (Ph.D.)
Kristian Paul, University of Delaware (Ph.D.)
Mihali Felipe, Yale University (Ph.D.)
Woh-jer Lee, California Institute of Technology (Ph.D.)

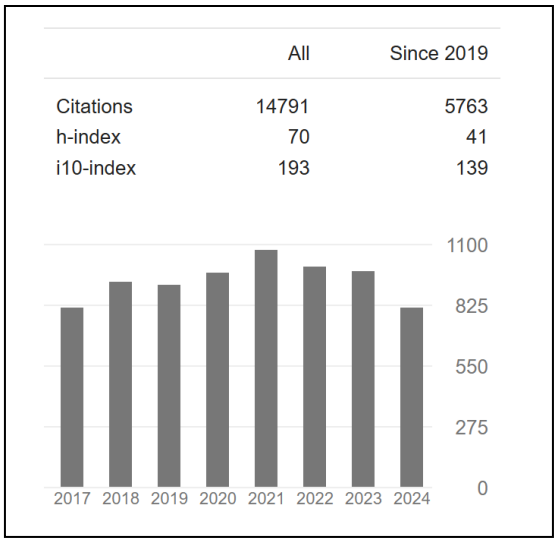
Undergraduate Students

Caress Riddell, The University of Texas at El Paso
Michael LaCroce, T. Blake Weiss, Virgil Gibilterra, Tiffany Zak, Stephanie Wexler, Alison Craven, Kim Kline, Brad Smoyer, Vikki Vry, Kim Salandro, The Pennsylvania State University
Grisselle Ortiz, University of Puerto Rico
Erin Carlson, Franklin & Marshall College
Tim Tambach, University of Amsterdam
Bao N. Nguyen, San Diego State University
Lynnette M. Schroeter, University of California, San Diego
Mika J. Itoh, University of San Diego

Postdoctoral Associates:

Jason Boettger, UTEP
Hui Yang, Heath Watts, Michael Mrozik, Lara Kabalan, Masoud Aryanpour, Qing Zhu, Louise Criscenti, Chad Trout, Jayakumar Narayanasamy, The Pennsylvania State University
Andrei Bandura, St. Petersburg State University, Russia
C. Ignacio Sainz-Diaz, Dept. of Earth Sciences and Environmental Chemistry, Spain
Andrew Zimmermann, The Pennsylvania State University
Paranthaman Selvarengan, Universite de Rennes

Publications



Google Scholar as of 11/15/2024

1. Cosgrove D.J., Dupree P., Gomez E.D., Haigler C.H., Kubicki J.D., Zimmer J. (2024) How many glucan chains form plant cellulose microfibrils? A mini review. *Biomacromolecules,* https://doi.org/10.1021/acs.biomac.4c00995.
2. Ilgen A.G., Borguet E., Geiger F.M., Gibbs J.M., Grassian V.H., Jun Y.S., Kabengi N., Kubicki J.D., (2024) Bridging molecular-scale interfacial science with continuum-scale models. *Nature Communications*, 15, 5326.
3. Barreto M.S.C., Elzinga E.J., Kubicki J.D., Sparks D.L. (2024) A multi-scale assessment of the impact of salinity on the desorption of chromate from hematite: Sea level rise implications. *Journal of Hazardous Materials,* 133041.
4. Watts H.D., Kubicki J.D., Pedentchouk N., Freeman K.H. (2024) Position-specific ^{2}H/H equilibrium isotopic fractionation factors in alkane, alkene and aromatic molecules: A density functional theory approach. *ACS Earth and Space Chemistry*, 8, 21-35.
5. Namayandeh, A., Borkiewicz, O., Bompoti, N., Watson, S., Kubicki, J., Chrysochoou, M., Michel, F. M. (2023) Effects of Oxyanion Surface Loading on the Rate and Pathway of Ferrihydrite Transformation. *ACS Earth and Space Chemistry*, 7, 2154-2165.
6. Machesky M.L., Kubicki J.D., Palmer D.A., Wesolowski D.J. (2023) Zn^{2+}, Co^{2+} and Ni^{2+} adsorption at the rutile-water interface to 250°C. *ACS Earth & Space Chemistry*, doi.org/10.1021/acsearthspacechem.3c00151.
7. Sit I., Young M.A., Kubicki J.D., Grassian V.H. (2023) Distinguishing different surface interactions for nucleotides adsorbed onto hematite and goethite particle surfaces through ATR-FTIR spectroscopy and DFT calculations. *Phys. Chem. Chem. Phys*. 25, 20557-20566
8. Banuelos J.L. Borguet E., Brown G.E., et al. (2023) Oxide- and Silicate-Water Interfaces and their Roles in Technology and the Environment. *Chemical Reviews*. (Co-lead author)
9. Del Mundo J., Rongpipi S., Yang H., Ye D., Kiemle S., Moffitt S., Troxel C., Toney M., Zhu C., Kubicki J.D., Cosgrove D., Gomez E., and Gomez E. (2023) Grazing-incidence diffraction reveals cellulose and pectin organization in hydrated plant primary cell wall. *Scientific Reports*, 13, 5421.
10. Boettger J.D., Neubauer, C., Kopf, S., Kubicki, J.D. (2022) Microbial Denitrification: Active Site and Reaction Path Models Predict New Isotopic Fingerprints. *ACS Earth & Space Chemistry*, 6 (11), 2582-2594.
11. Al-Abadleh H.A., Kubicki J., Meskhidze N. (2023) A perspective on iron (Fe) in the atmosphere: air quality, climate, and the ocean. *Environmental Science: Processes & Impacts*, 2022, DOI: 10.1039/D2EM00176D.
12. Watts H.D., Kubicki J.D., Kabengi N. (2022) Connecting thermodynamics of alkali ion exchange on the quartz (101) surface with density functional theory calculations. *The Journal of Physical Chemistry A*, **126**, 4286-4294. https://doi.org/10.1021/acs.jpca.2c02697
13. Ridley M.K., Machesky M.L., Kubicki J.D. (2022) Ion and Particle Size Effects on the Surface Reactivity of Anatase Nanoparticle–Aqueous Electrolyte Interfaces:

Experimental, Density Functional Theory, and Surface Complexation Modeling Studies. *Minerals*, **12**, 907. https://doi.org/10.3390/min12070907
14. Ohno T., Amirbahman A., Kubicki J.D. (2022) Molecular Orbital Study of Fe(II) and Fe(III) Complexation with Salicylate and Citrate Ligands: Implications for Soil Biogeochemistry. *Soil Science Society of America Journal*, DOI: 10.1002/saj2.20339.
15. Yuan K., Rampal N., Fenter P., Kubicki J.D., Stack A.G., Irle S. (2021) Density functional tight-binding simulations reveal the presence of surface defects on the quartz (101)-water interfaces. *The Journal of Physical Chemistry C*. /doi.org/10.1021/acs.jpcc.1c03689.
16. Boettger J.D., Kubicki, J.D. (2021) Equilibrium and Kinetic Isotopic Fractionation in the CO_2 Hydration and Hydroxylation Reactions: Analysis of the Role of Hydrogen-bonding via Quantum Mechanical Calculations. *Geochimica Cosmochimica Acta*, 292: 37–63.
17. Fox A., Boettger J.D., Kubicki J.D., Freeman K.H. (2020) Density Functional Theory Predictions of Non-covalent Hydrogen Isotope Effects during Octane Sorption to a Kaolinite Surface. *ACS Earth and Space Chemistry*, 4, 1756-1764 doi: 10.1021/acsearthspacechem.0c00148.
18. Kubicki J.D., Ohno T. (2020) Integrating density functional theory modeling with experimental data to understand and predict sorption reactions: Exchange of salicylate for phosphate on goethite. *Soil Systems*, 4 (2), 27.
19. Singh A., Kwansa A.L., Kim H.S., Williams J.T., Yang H., Li N.K., Kubicki J.D., Roberts A.W., Haigler C.H., Yingling Y.G. (2020) In silico structure prediction of full-length cotton cellulose synthase protein (GhCESA1) and its hierarchical complexes, *Cellulose*, 27:5597–5616. https://doi.org/10.1007/s10570-020-03194-7.
20. Ohno T., Kubicki J.D. (2020) Adsorption of organic acids and phosphate to an iron (oxyhydr)oxide mineral: A combined experimental and density functional theory study. *The Journal of Physical Chemistry A*, **124**, 3249-3260. https://dx.doi.org/10.1021/acs.jpca.9b1204.
21. Soldoozy S., Trinh A., Kubicki J.D., Al-Abadleh H.A. (2020) In situ and real-time ATR-FTIR temperature-dependent adsorption kinetics coupled with DFT calculations of dimethylarsinate and arsenate on hematite nanoparticles. *Langmuir*, **35**, 4299-4307. https://dx.doi.org/10.1021/acs.langmuir.0c00252.
22. Yang H., Kubicki J.D. (2020) A density functional theory study on the shape of the primary cellulose microfibril in plants: Effects of C6 exocyclic group conformation and H-bonding. *Cellulose*, 1-14.
23. Ajayi O.A., Kubicki J.D. (2020) Interfacial energies of supercritical CO_2 and water with 2:1 layered silicate surfaces: a density functional theory study. *Applied Geochemistry*, 114, 104514.
24. Boettger J., Kubicki J.D. (2019) Evaluating computational chemistry methods for isotopic fractionation between CO_2(g) and H_2O(g). *J. Chem. Inf. Modeling*, *59*(11), 4663-4677.
25. Yang H., Watts H.D., Gibilterra V.T., Blake W., Petridis L., Cosgrove D.J., Kubicki J.D. (2019) Quantum calculations on plant cell wall component interactions. *Interdisciplinary Sciences: Computational Life Sciences*, **11**, 485-495. doi.org/10.1007/s12539-018-0293-4.
26. Watts H.D., O'Day P.A., Kubicki J.D. (2019) Gibbsite (100) and Kaolinite (100) Sorption of Cadmium(II): a Density Functional Theory and XANES Study of Structures and Energies. *The Journal of Physical Chemistry A*, **123**, 6319-6333.
27. Yang H., McManus J., Oehme D., Singh A., Yingling Y.G., Tien M., Kubicki J.D. (2019) Simulations of cellulose synthesis initiation and termination in bacteria. *Journal of Physical Chemistry B*, **123**, 3699-3705.
28. Allen N., Dai C., Hu Y., Kubicki J.D., Kabengi N. (2019) Adsorption study of Al^{3+}, Cr^{3+} and Mn^{2+} onto quartz and corundum using flow microcalorimetry, quartz crystal microbalance, and density functional theory. *ACS Earth and Space Chemistry*, DOI: 10.1021/acsearthspacechem.8b00148.
29. Kubicki J.D., Watts H.D. (2019) Quantum mechanical modeling of the vibrational spectra of minerals with a focus on clays. *Minerals*, **9**, 141; doi:10.3390/min9030141
30. Bracco J.N., Lee S.S., Stubbs J.E., Eng P.J., Jindra S., Warren D.M., Kommu A., Fenter P., Kubicki J.D., Stack A.G. (2019) Simultaneous adsorption and incorporation of Sr^{2+} at the barite (001)-water interface. *The Journal of Physical Chemistry C*, **123**, 1194-1207.
31. Shrestha U.R., Smith S., Pingali S.V., Yang H., Zahran M., Breunig L., Wilson L.A., Kowali M., Kubicki J.D., Cosgrove D.J., O'Neill H.M., Petridis L. (2019) Arabinose substitution effect on xylan rigidity and self-aggregation. *Cellulose*, **26**, 2267-2278.
32. Makarem M., Lee C.M., Kafle K., Huang S., Chae I., Yang H., Kubicki J.D., Kim S.H. (2019) Probing cellulose structures with vibrational spectroscopy. *Cellulose*, **26**, 35-79.

DOI:10.1007/s10570-018-2199-z
33. Khan N.A., Johnson M.D., Kubicki J.D., Holguin O., Dungan B., Carroll K.C. (2019) Cyclodextrin-enhanced 1,4-dioxane treatment kinetics with TCE and 1,1,1-TCA using aqueous ozone, *Chemosphere*, **219**, 335-344, doi.org/10.1016/j.chemosphere.2018.11.200.
34. McManus J.B., Wilson L., Yang H., Kubicki J.D., Tien M. (2018) Kinetic analysis of cellulose synthase of *Gluconacetobacter hanseii* in whole cells and pure form. *Enzyme and Microbial Technology*, **119**, 24-29.
35. Kubicki J.D., Yang H., O'Neill H., Sawada D., Cosgrove D. (2018) The shape of native plant cellulose microfibrils. *Scientific Reports*, **8**, Article number: 13983.
36. Oehme D.P., Yang H., Kubicki J.D. (2018) An evaluation of the structures of cellulose generated by the CHARMM force field: comparisons to *in planta* cellulose. *Cellulose*, https://doi.org/10.1007/s10570-018-1793-4
37. Kubicki J.D., Kabengi N., Chrysochoou M., Bompoti N. (2018) Density functional theory modeling of chromate adsorption onto ferrihydrite nanoparticles. *Geochem. Trans.*, **19**, 8.
38. Yang H., Wang T., Oehme D., Petridis L., Hong M., Kubicki J.D. (2018) Structural factors affecting ^{13}C NMR chemical shifts of cellulose: a computational study. *Cellulose*, **25**, 23-36.
39. Borowski S.C., Biswakarma J., Kang K., Schenkeveld W.D.C., Hering J.G., Kubicki J.D., Kraemer S.M., Hug S.J. (2018) Structure and reactivity of oxalate surface complexes on lepidocrocite derived from infrared spectroscopy, DFT calculations, adsorption, dissolution and photochemical experiments. *Geochimica et Cosmochimica Acta*, **226**, 244-262.
40. McManus, J.; Yang, H.; Kubicki, J.D.; Tien, M. (2018) Initiation, Elongation and Termination of Bacterial Cellulose Synthesis. *ACS Omega*, **3**. 2690-2698.
41. Wang, Xi. Kubicki, J.D., Boily, J-F. Waychunas, G.A. Hu, Y. Feng, X., Zhu, M. (2018) Binding geometries of silicate species on ferrihydrite surfaces. *ACS Earth and Space Chemistry*, **2**, 125-134.
42. Harouaka K., Kubicki J.D., Fantle M.S. (2017) Effect of amino acids on the precipitation kinetics of Ca isotopic composition of gypsum. *Geochimica et Cosmochimica Acta*, **218**, 343-364.
43. Ling F.T., Post J.E., Heaney P.J., Kubicki J.D., Santelli C.M. (2017) Fourier-transform infrared spectroscopy analysis of triclinic and hexagonal birnessites. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, **178**, 32-46.
44. Hüffer T., Sun H., Kubicki J.D., Hofmann T., Kah M. (2017) Interactions between aromatic hydrocarbons and functionalized C60 fullerenes – insights from experimental data and molecular modeling. *Environmental Science: Nano*, **4**, 1045 - 1053.
45. Kubicki J.D., Tunega D., Kraemer S. (2017) A density functional theory investigation of oxalate and Fe(II) adsorption onto the (010) goethite surface with implications for ligand- and reduction-promoted dissolution. *Chemical Geology*, **464**, 14-22.
46. Kabengi N.J., Chrysochoou M., Bompoti N., Kubicki J.D. (2017) An integrated flow microcalorimetry, infrared spectroscopy and density functional theory approach to the study of chromate complexation on hematite and ferrihydrite. *Chemical Geology*, 464, 23-33. http://dx.doi.org/10.1016/j.chemgeo.2017.01.017
47. DelloStritto M.J., Kubicki J.D., Sofo J.O. (2016) Effect of ions on H-bond structure and dynamics at the quartz(101)-water interface. *Langmuir*, **32**, 11353-11365. DOI: 10.1021/acs.langmuir.6b01719
48. Alstadt V., Kubicki J.D., Freedman M.A. (2016) Competitive adsorption of acetic acid and water on kaolinite. *J. Phys. Chem. A*, **120**, 8339-8346.
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