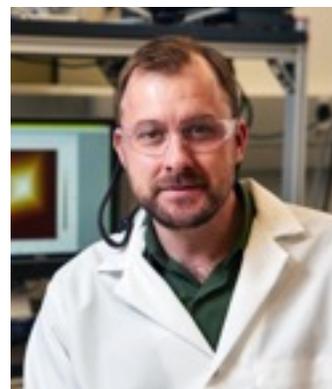


## ANDREW G. STACK

Senior R&D Staff  
Chemical Sciences Division  
Oak Ridge National Laboratory  
One Bethel Valley Road  
Bldg. 4100, Rm. C342, MS-6110  
Oak Ridge, TN 37831-6110  
Phone: 865-574-8450, Fax: 865-574-4961  
E-mail: [stackag@ornl.gov](mailto:stackag@ornl.gov)



### Professional Interests

Mineral surface chemistry, particularly mineral growth and dissolution. Chemical reaction kinetics and mechanisms. Fate and transport of contaminants.

### Educational Background

Ph.D. Geology	2002	University of Wyoming
M.S. Geology	1999	University of Wyoming
B.S. Geological Sciences: Geochemistry option	1997	Virginia Polytechnic Institute

### Employment History

Senior R&D Staff	Oak Ridge National Laboratory	2014-present
R&D Staff	Oak Ridge National Laboratory	2010-2013
Assistant Professor	Georgia Institute of Technology	2005-2010
Postgraduate Researcher	University of California, Davis	2002-2005
Graduate Research Assistant	University of Wyoming	1997-2002
Temporary Scientist Level I	Shepherd-Miller Inc.	1998
Graduate Teaching Assistant	University of Wyoming	1997
Hydrologist	U.S. Geological Survey	1994-1997

### Honors & Awards

Outstanding Contributions to Geosciences Research Award (2014). U.S. DOE Basic Energy Sciences, Geosciences Program  
Profile featured at ORNL web-site ([Part I](#), [Part II](#)), [STEM Magazine](#) (2015)  
Profile featured in American Chemical Society's "[College-To-Career](#)" web-site  
Award for One of Top 14 Technical Presentations (out of > 300), Twelfth Annual Conference on Carbon Capture, Utilization & Sequestration. Pittsburgh, PA, May 13-16, 2013  
ORNL Incentivized Performance Award (2014)  
ORNL Supplemental Performance Awards (2013, 2012, 2011)  
Mineralogical Society of America Undergraduate Award (1997)  
U.S. Department of Interior On-the-Spot Award (1996)  
Finalist for [Asylum Research AFM Image Contest](#)

### Professional Activities

Past Division Chair for the Geochemistry Division of the American Chemical Society (2015), Division Chair (2014), Program Chair (2013), Program-Chair Elect (2012)

Editorial Board Member, *Geochemical Transactions* (2013-2015)  
Member of Adjunct Graduate Faculty, Wright State University (2013-present)  
Member of ORNL Research Conflict of Interest Committee (2015-present)  
Attended ORNL Developing Leadership Potential (2015), Management Boot Camp (2013) courses  
Contributed to Department of Energy, Basic Energy Sciences workshops and reports on Subsurface Technology and Engineering Research Program (SubTER) and a new Grand Challenge for Subsurface Science (2015)  
Member of ORNL Center for Accelerated Materials Modeling Scientific Advisory Committee (2015-present)  
Organizer of Geochemistry Division Programming at National American Chemical Society conferences (fall 2013, spring 2014)  
Organizer of symposia at Pacificchem (2015), semi-annual National American Chemical Society conferences (2×spring 2015, spring 2014, spring 2013, fall 2013), V. M. Goldschmidt Geochemical Society conferences (2×2015, 2012, 2×2010, 2009, 2007, 2005)  
Member of the Proposal Study Council (2013) & Proposal Study Panel (2012) for the Molecular Foundry, a DOE Nanoscale Science Research Center  
Served on U.S. National Science Foundation Geobiology and Low Temperature Aqueous Geochemistry review panels (2012, 2011, 2009)  
Served on review panel for the U.S. Department of Energy Biological and Environmental Research Program triennial review of the Environmental Molecular Sciences Laboratory at Pacific Northwest National Laboratory (2011)  
Member: *American Chemical Society*; *Geochemical Society*

### **Publications** ([h-index = 16](#))

1. Stack, A. G. (2015) Precipitation in Pores: A Geochemical Frontier. *Rev. Mineral. Geochem.* 80, 165-190 [DOI: 10.2138/rmg.2015.80.05](https://doi.org/10.2138/rmg.2015.80.05)
2. Godinho, J. R. A.; **Stack, A. G.** (2015) Growth kinetics and morphology of barite crystals derived from face-specific growth rates. *Cryst. Growth Des.* 15, 2064-2071 [DOI: 10.1021/cg501507p](https://doi.org/10.1021/cg501507p)
3. **Stack, A. G.**; Kent, P. R. C. (2015) Geochemical Reaction Mechanism Discovery from Molecular Simulation. *Environ. Chem.* 12, 20-32. [DOI: 10.1071/EN14045](https://doi.org/10.1071/EN14045)
4. Hatzell, M. C.; Raju, M.; Watson, V. J.; **Stack, A. G.**; van Duin, A. C. T.; Logan, B. E. (2014) Effect of Strong Acid Functional Groups on Electrode Rise Potential in Capacitive Mixing by Double Layer Expansion. *Environ. Sci. Technol.* 48, 14041-14048. [DOI: 10.1021/es5043782](https://doi.org/10.1021/es5043782)
5. Bracco, J. N.; **Stack, A. G.**; Higgins, S. R. (2014) Magnesite step growth rates as a function of the aqueous magnesium-to-carbonate ratio. *Cryst. Growth Des.* 14, 6033-6040. [DOI: 10.1021/cg501203g](https://doi.org/10.1021/cg501203g)
6. **Stack, A. G.**; Fernandez-Martinez, A.; Allard, L. F.; Bañuelos, J. L.; Rother, G.; Anovitz, L. M.; Cole, D. R.; Waychunas, G. A. (2014) Pore-Size-Dependent Calcium Carbonate Precipitation Controlled by Surface Chemistry. *Environ. Sci. Technol.* 48, 6177-6183.

7. **Stack, A. G.** (2014) Next generation models of carbonate mineral growth and dissolution. *Greenhouse Gases: Sci. Technol.* **4**, 278-288.
8. Gazzè, S. A.; **Stack, A. G.**; Ragnarsdottir, K. V.; McMaster, T. J. (2014) Chlorite topography and dissolution of the interlayer studied with Atomic Force Microscopy. *Am. Mineral.* **99**(1), 128-138.
9. Qin, L.; Zhang, W.; Lu, J.; **Stack, A.G.**; Wang, L. (2013) Direct Imaging of Nanoscale Dissolution of Dicalcium Phosphate Dihydrate by an Organic Ligand: Concentration Matters. *Environ. Sci. Technol.* **47**(23), 13365-13374.
10. Wang, H.-W.; Anovitz, L. M.; Burg, A.; Cole, D. R.; Allard, L. F.; Jackson, A. J.; **Stack, A. G.**; Rother, G. (2013) Multi-scale characterization of pore evolution in a combustion metamorphic complex, Hatrurim basin, Israel: Combining (ultra) small-angle neutron scattering and image analysis. *Geochim. Cosmochim. Acta*, **121**, 339-362.
11. Bracco, J. N.; **Stack, A. G.**; Steefel, C. I. (2013) Upscaling Calcite Growth Rates From the Meso- to the Macro- Scale. *Environ. Sci. Technol.*, **47**, 7555-7562. [DOI: 10.1021/es400687r](https://doi.org/10.1021/es400687r)
12. **Stack, A. G.**; Gale, J. D.; Raiteri, P. (2013) Virtual Probes of Mineral–Water Interfaces: The More Flops, the Better! *Elements*, **9**, 211-216.
13. Rother, G.; Ilton, E. S. Wallacher, D.; Hauß, T.; Schaefer, H. T.; Qafoku, O.; Rosso, K. M.; Felmy, A. R.; Krukowski, E. G.; **Stack, A. G.**; Grimm, N.; Bodnar, R. J. (2013) CO<sub>2</sub> sorption to subsingle hydration layer montmorillonite clay studied by excess sorption and neutron diffraction measurements. *Environ. Sci. Technol.*, **47**, 205-211.
14. Bracco, J. N.; Grantham, M. C.; **Stack, A. G.** (2012) Calcite growth rates as a function of aqueous calcium-to-carbonate ratio, saturation index, and inhibitor concentration: Insights into the mechanism of reaction and poisoning by strontium. *Cryst. Growth Des.* **12**, 3540-3548. [DOI: 10.1021/cg300350k](https://doi.org/10.1021/cg300350k)
15. **Stack, A. G.**; Raiteri, P.; Gale, J. D. (2012) Accurate rates of the complex mechanisms for growth and dissolution of minerals using a combination of rare event theories. *J. Am. Chem. Soc.* **134**, 11-14.
16. Zhang, W.; **Stack, A. G.**; Chen, Y. (2011) Interaction Force Measurement between *E. coli* Cells and Nanoparticles Immobilized Surfaces by Using AFM. *Colloids Surf. B: Biointerfaces* **82**, 316-324.
17. **Stack, A. G.**; Grantham, M. C. (2010) The growth rate of calcite steps as a function of aqueous calcium-to-carbonate ratio: independent attachment and detachment of calcium and carbonate ions. *Cryst. Growth Des.* **10**, 1409-1413.
18. Zhang, M.; Burns, J. L.; DiChristina, T. J.; **Stack, A. G.** (2010) Attachment isotherms of *Shewanella oneidensis* to amorphous iron (oxy)(hydr)oxides. *Envi. Sci. Technol.* **44**, 1602-1609.
19. Wang, X.; Ingall, E.; Lai, B.; **Stack, A. G.** (2010) Self-assembled Monolayers as Templates for Heme Crystallization. *Cryst. Growth Des.* **10**, 798-805.
20. **Stack, A.G.** (2009) Molecular Dynamics Simulations of Solvation and Kink Site Formation at the {001} Barite-Water Interface. *J. Phys. Chem. C*, **113**, 2104-2110.

21. Zhang, M.; Dale, J. R.; DiChristina, T. J.; **Stack, A. G.** (2009) Dissolution morphology of iron (oxy)(hydr)oxides exposed to the dissimilatory iron reducing bacterium *Shewanella oneidensis* MR-1. *Geomicrobiol. J.*, **26**, 83-92.
22. Wigginton, N. S.; Rosso, K. M.; **Stack, A. G.**; Hochella, Jr. M. F. (2009) Long-Range Electron Transfer Across Cytochrome-Hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) Interfaces. *J. Phys. Chem. C*, **113**, 2096-2103.
23. **Stack, A.G.**; Rustad, J. R. (2007) Structure and Dynamics of Water on Aqueous Barium Ion and the {001} Barite Surface. *J. Phys. Chem. C*, **111**, 16387-16391.
24. Rustad, J. R.; **Stack, A. G.** (2006) Molecular dynamics calculation of the activation volume for water exchange on Li<sup>+</sup>. *J. Am. Chem. Soc.*, **128**, 14778-14779.
25. **Stack A. G.**, Rustad J. R., Casey W. H. (2005) Modeling water exchange on an aluminum polyoxocation. *J. Phys. Chem. B (Letters)* **109**, pp. 23771-23775.
26. **Stack A. G.**, Rustad J. R., Land T. A., De Yoreo J. J., Thomas T. N. & Casey W. H. (2004) The growth morphology of the {100} surface of KDP (Archerite) on the molecular scale. *J. Phys. Chem. B.* **108**, pp. 18284-18290.
27. **Stack A. G.**, Erni R., Browning N. D. & Casey W. H. (2004) Pyromorphite growth *in situ* on lead sulfides. *Envi. Sci. Technol.* **38**, pp. 5529-5534.
28. **Stack A. G.**, Eggleston C. M. & Engelhard M. H. (2004) Reaction of hydroquinone with hematite I: Electrochemical scanning tunneling microscopy and X-ray photoelectron spectroscopy. *J. Coll. Int. Sci.*, **274**, pp. 433-441.
29. **Stack A. G.**, Rosso K. M., Smith D. M. A. & Eggleston C. M. (2004) Reaction of hydroquinone with hematite II: Calculation of the electron transfer rate and comparison to the dissolution rate. *J. Coll. Int. Sci.*, **274**, pp. 442-450.
30. Eggleston C.M., **Stack A.G.**, Rosso K.M. & Bice A.M. (2004) Adatom Fe(III) on the hematite surface: Observation of a key reactive surface species. *Geochem. Trans.* **5**, 2, pp. 33-40.
31. Eggleston C. M., **Stack A. G.**, Rosso K. M., Higgins S. R., Bice A. M., Boese S. W., Pribyl R. D. & Nichols J. J. (2003) The structure of hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) (001) surfaces in aqueous media: Scanning tunneling microscopy and resonant tunneling calculations of coexisting O and Fe terminations. *Geochim. Cosmochim. Acta.* **67**, 5, pp. 985-1000.
32. **Stack A. G.**, Higgins S.R. & Eggleston C.M. (2003) Response to comment on "Point of zero charge of a corundum-water interface probed with optical second harmonic generation (SHG) and Atomic Force Microscopy (AFM): New approaches to oxide surface charge. *Geochim. Cosmochim. Acta.* **67**, 2, pp. 321-322
33. Higgins S. R., **Stack A. G.**, Knauss K. G., Eggleston C. M. & Jordan G. (2002) Probing molecular scale adsorption and dissolution-growth processes using nonlinear optical and scanning probe methods suitable for hydrothermal applications. In *Water-Rock Interactions, Ore Deposits, and Environmental Geochemistry: A Tribute to David A. Crerar*, Special Publication No. 7 (ed. R. Hellmann and S. A. Wood), pp. 111-128. The Geochemical Society.
34. **Stack A. G.**, Higgins S.R. & Eggleston C.M. (2001) Point of zero charge of a corundum-water interface probed with optical Second Harmonic Generation (SHG) and Atomic

Force Microscopy (AFM): New approaches to oxide surface charge. *Geochim. Cosmochim. Acta* **65**, 18, pp. 3055-3063.

35. Higgins, S. R.; Stack, A. G.; Eggleston, C. M.; Afonso, M. D. S. (1998) Proton and ligand adsorption at silica-and alumina-water interfaces studied by optical second harmonic generation (SHG). *Mineral. Mag.*, **62**, 616-617.

### Research Grants and Contracts

Principal Investigator, “Atoms- to Pore-Scale Geochemical Reactions” , U.S. DOE, Office of Basic Energy Sciences, 10/1/2015-9/30/2018, \$1,700k/yr. 6 person-months per year, **current**.

ORNL Team Lead, “Center for Nanoscale Control of Geologic CO<sub>2</sub>, an Energy Frontier Research Center” U.S. DOE, Office of Basic Energy Sciences, 8/01/14 – 09/30/18, \$3,200k/yr (ORNL portion \$490k/yr). 3 person-months per year, **current**.

Project 1.1.1 Team Lead (2015-present), also Team Member (2013-2015). “Critical Materials Institute.” U.S. DOE, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office. 6/29/2013 - 6/30/2018, \$25,000k/yr (project 1.1.1 portion \$850k/yr). 3 person-months per year, **current**.

Principal Investigator “Reducing Environmental Impacts of Hydrofracturing by Subsurface Co-Precipitation of Barium and Radium.” ORNL Laboratory Directed Research and Development. \$388k/yr. 03/15/13 - 03/14/15. 2 person-months per year.

Subtask 2 leader, “Geochemical Equilibria and Reaction Dynamics: Atomic- to Pore-Scale Processes” U.S. DOE, Office of Basic Energy Sciences, Geosciences program, 10/1/2012 – 10/2/2015, \$1,700,000/yr (Subtask 2 portion \$580k/yr). 3 person-months per year.

Team Member, “Improving Chemical Separations through Understanding Weak Interactions” U.S. DOE, Office of Basic Energy Sciences, 8/1/12 – 7/31/15, \$400k/yr. 2 person-months per year.

ORNL team lead (2013-2014), also Team Member (2010-2013), “Center for Nanoscale Control of Geologic CO<sub>2</sub>, an Energy Frontier Research Center” U.S. DOE, Office of Basic Energy Sciences, 10/01/13 – 8/31/14, \$20,000,000 (ORNL portion \$550k/yr). 3 person-months per year.

Subtask 1 leader, “Structure and Dynamics of Earth Materials, Interfaces and Reactions” U.S. DOE, Office of Basic Energy Sciences, Geosciences program, 10/1/2009 – 9/30/2012, \$5,595,000. 5.2 person-months per year.

Principal Investigator, “Testing Molecular Mechanisms for Growth and Dissolution Reactions on Calcite Surfaces” U.S. NSF, Earth Sciences Directorate, Geobiology and Low Temperature Aqueous Geochemistry program, 08/01/07 - 07/31/10, \$219,385.

Principal Investigator, “Reaction mechanisms for barite dissolution and growth.” U.S. DOE, Basic Energy Sciences Program, Geosciences Subprogram, 08/01/07 - 07/31/2009, \$209,747.

co-Investigator, “Characterization of Mineral Dust Aerosols to Improve Predictions of Their Impact on the Radiative Balance of the Atmosphere.” U.S. NOAA, 04/01/07 - 03/31/10, \$314,741.

## Invited Talks and Symposia

1. “Mineral Precipitation Reactions from the Atomic- to Pore Scales.” Departmental Colloquium, Pennsylvania State University, Department of Geosciences, Oct. 6th, 2015.
2. “Precipitation in Pores” Keynote address, Pore Scale and Nano-Confined Geochemical Processes, V. M. Goldschmidt Conference, Aug., 20, 2015.
3. “Atomic- to Pore-Scale Understanding and Prediction of Mineral Precipitation.” Departmental seminar, *University of Houston, Dept. of Civil and Environ. Engineering*. Nov. 24, 2014.
4. “Atomic- to Pore-Scale Probes and Predictions of Mineral Reactivity.” *U.S. DOE Basic Energy Sciences, Geosciences Program*, Research PI Meeting, May 14-16, 2014.
5. “Atomic-scale to Mesoscale simulation of mineral growth and dissolution reactions.” *247<sup>th</sup> Meeting of the American Chemical Society*, Dallas, TX, March 16-20, 2014.
6. “Mechanisms and Rates of Reaction for Crystallization from the Atomic to Macroscopic Scales: Simulation, Theory and Experiment.” *Advanced Photon Source User Seminar Series*, Nov. 15, 2013.
7. “Upscaling Carbonate Mineral Growth Rates From the Nano- to Pore- Scales and Beyond: Current Progress and Future Directions.” *Twelfth Annual Conference on Carbon Capture, Utilization & Sequestration*. Pittsburgh, PA, May 13-16, 2013.
8. “Mechanisms and Rates of Reaction at Mineral-Water Interfaces from the Atomic to Pore Scales: Simulation, Theory and Experiment.” *Division Seminar, Chemical Sciences and Materials Sciences Divisions, ORNL*. April 17, 2013.
9. “Fast Water Exchange on a Mineral Surface Measured by Quasi-Elastic Neutron Scattering (QENS) and Classical Molecular Dynamics (MD).” Session on “Approaching the Surface: Interrogating Chemical Interactions at the Mineral-Water Interface.” *245<sup>th</sup> Meeting of the American Chemical Society*, New Orleans, LA, April 7-11, 2013
10. “Nucleation and Growth of Minerals (Calcium Carbonate) in Porous Media” *U.S. DOE BES Geosciences Workshop* on “Reaction and Transport within Internal Domains of Porous Media” San Francisco, December 1-2, 2012.
11. “Calcite Growth from the Molecular Scale.” Session on Physicochemical constraints of the marine carbonate system: recent insights into the reactivity of carbonate minerals in aqueous solutions. *Goldschmidt 2012*, Montréal, Canada, June 24-29, 2012.
12. “Molecular level mechanisms of mineral growth and dissolution.” *Seminar for Geophysical Laboratory*. *Carnegie Institute*, Washington, D. C., January 9, 2012.
13. "Rates of mineral growth and dissolution reactions from molecular dynamics." Session on Large and Complex Atomistic Systems: Physics, Algorithms and Hardware. *Goldschmidt 2011*, Prague, Czech Republic, August 14-19, 2011.
14. “Interaction between iron respiring bacteria and iron (oxy)(hydr)oxides.” Departmental seminar at *Washington University at St. Louis*, Department of Earth and Planetary Sciences. September 17, 2009.

15. "Reactions controlling step movement during mineral dissolution and growth" Session on Molecular Computational Geochemistry for Water-Rock Interactions. *237th Meeting of the American Chemical Society*, Salt Lake City, March 22-26, 2009
16. "Applications of electrochemical scanning tunneling microscopy to adsorption and thin films in geochemical systems." Session on Advanced Approaches to investigating Adsorption at the solid–Water interface., *235th Meeting of the American Chemical Society*, New Orleans, LA, April 6-10, 2008
17. "Comparison of computational and experimental barite-water interface structures and kinetics." Session on Physical chemistry of environmental interfaces. *235th Meeting of the American Chemical Society*, New Orleans, LA, April 6-10, 2008
18. "Water structure on aqueous ions and barite-water interfaces." Division of Colloid and Surface Chemistry. *235th Meeting of the American Chemical Society*, New Orleans, LA, April 6-10, 2008.
19. "Prediction of ligand exchange and crystal growth kinetics using atomistic computational methods. Seminar. *William R. Wiley Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory*. Richland, WA, January 14th, 2008.
20. "Modeling water exchange on an aluminum polyoxocation." Seminar. *Chemical and Analytical Sciences Division, Oak Ridge National Laboratory*. Oak Ridge, TN, October 10th, 2005.

#### **Advisees**

##### Oak Ridge National Laboratory

- Ms. Anna Wanhala, Bredesen Center Ph.D. Student (2015-present)  
 Dr. Hsiu-Wen Wang, Joint Institute for Neutron Scattering Researcher (2014-present)  
 Dr. Michael C. Cheshire, Post-Doctoral Researcher (2014-present)  
 Dr. José R. A. Godinho, Post-Doctoral Researcher (2013-2015)  
 Dr. Alexander D. Gordon, Post-Doctoral Researcher (2013-2014)

##### Georgia Institute of Technology

- Ms. Jacquelyn N. Bracco, undergraduate & M.S. student. (graduated spring 2012)  
 Mr. Davis (Morgan) Warren, M.S. student (graduated spring 2011)  
 Ms. Cynthia M. Jackson, undergraduate student. (graduated spring 2011)  
 Dr. Mengni Zhang, Ph.D. (Received departmental best paper award, 2009; graduated fall, 2010)  
 Dr. Xuefeng Wang, postdoctoral researcher (2008-2010)  
 Mrs. Lindsay Wallace, non-thesis MS. (graduated spring 2010)  
 Mr. John Revere Brand, undergraduate student. (graduated spring 2008)

#### **Academic Committee Service**

##### Dissertation Committees - University of Tennessee, Knoxville

- Victoria DiStefano, Ph.D. (expected spring 2017)  
 Anna Wanhala, Ph.D., Committee chair (expected spring 2019)

Dissertation/Thesis Committees - Wright State University

Jacquelyn N. Bracco, Ph.D. (graduated fall 2015)

Dennis Lenaerts, M.S. (spring 2013)

Department Committees - Georgia Institute of Technology

Co-Chair, Graduate Student Acceptance Committee (2009/2010).

Graduate Student Acceptance Committee (2005-2009)

Undergraduate Curriculum Committee (2006/2007)

EAS Faculty Search Committee (2006/2007)

Graduate Student Thesis Committees (2005-2010).

**Courses Taught**

Georgia Institute of Technology, School of Earth and Atmospheric Sciences

<b>Semester</b>	<b>Course</b>	<b>Title</b>	<b>Enrollment</b>
Spring, 2010	EAS 8803	Special Study: The Origin of Life	1
Fall, 2009	EAS 4110	Resources, Energy and the Environment	20
Fall, 2009	EAS 8803	Mineral Surface Geochemistry	10
Fall, 2009	EAS 4900	Special Study: C++ for Geochemists	3
Fall, 2008	EAS 4803/8803	Resources, Energy and the Environment	28
Spring, 2008	EAS 4803/8803	Water Quality Modeling	4
Fall, 2007	EAS 4803	Resources, Energy and the Environment	18
Spring, 2007	EAS 4803/8803	Water Quality Modeling	5
Fall, 2006	EAS 8803	Mineral Surface Geochemistry	9
Fall, 2005	EAS 4803/8803	Water Quality Modeling	5

University of Wyoming, Department of Geology and Geophysics

<b>Semester</b>	<b>Course</b>	<b>Title</b>	<b>Enrollment</b>
Summer, 2001	GEOL/ASTR 1070	The Earth: Its Physical Environment (U. Wyo. Wind River Reservation Extension)	6