

Zhou Yu, Ph.D.

Postdoc Research Associate
Physics and Chemistry of Materials Group
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RESEARCH GOAL

My research goal is to establish simulation and theory-driven approaches (e.g., density functional theory calculations, molecular dynamics simulations, machine learning techniques, etc.) to understand and predict bulk and interfacial physicochemical properties (e.g., structure, transport, mechanical, chemical, and electrochemical, etc.) of advanced functional materials including electrolytes, membranes, colloids, porous materials, etc. in multiple spatial scales ranging from molecular (\AA) to nanometric domains (μm) and time scales ranging from solvation shell exchange (ps) to assembly (μs).

RESEARCH EXPERTISE AND INTERESTS

1. *Multiscale simulations* including molecular dynamics simulations, density functional theory calculations, and machine learning techniques on *advanced functional materials*
2. *Structure-property-performance relationships* in novel battery electrolytes including *liquid* electrolytes and *polymer* electrolytes
3. *Interfacial and transport phenomena* involved in energy storage and conversion process

EDUCATION

Ph.D. in Mechanical Engineering, 12/2018

Virginia Tech, Blacksburg, VA, USA GPA: 3.85/4.0

- Dissertation: "Molecular structure and dynamics of novel polymer electrolytes featuring coulombic liquids"
- Advisor: [Prof. Rui Qiao](#)

M.E. in Engineering Thermophysics, 6/2015

Shandong University, Jinan, China GPA: 88.20/100 Rank: 2/142

- Thesis: "Experimental investigation of a dynamic cyclone on gas-solid separation"
- Advisor: Prof. Chunyuan Ma

B.E. in Thermal Energy and Power Engineering, 6/2012

Shandong University, Jinan, China GPA: 88.11/100 Rank: 18/213

RESEARCH EXPERIENCES

Los Alamos National Laboratory, Los Alamos, NM 11/2021 – Present

Postdoc Research Associate

Advisor: [Dr. Enrique R. Batista](#), [Dr. Danny Perez](#), [Dr. Ping Yang](#)

- Explore the separation process of rare earth elements using ionic liquids
- Investigate the solvation free energy of rare earth elements in water and ionic liquids

- Screen ionic liquids for separation using Multi-objective Bayesian Optimization

Argonne National Laboratory, Lemont, IL

2/2019 – 11/2021

Postdoctoral Appointee

Advisor: [Dr. Lei Cheng](#), Mentor: [Dr. Subramanian Sankaranarayanan](#)

- Elucidated the solution structure transition in salt-concentrated electrolytes
- Explored the transport mechanism and correlated transport properties in salt-concentrated electrolytes
- Investigated the effects of supporting salts on solvation and redox potential of redox-active organic molecules used in redox flow batteries
- Studied the bulk and interfacial redox pathway of lithium-sulfur battery electrolytes
- Developed the machine learning force fields of multivalent metallic cations in aqueous solutions

Virginia Tech, Blacksburg, VA

8/2015 – 12/2018

Research Assistant

- Explored the molecular structure and dynamics of polymeric ion gel and nanoscale ionic materials
- Investigated the effects of electrified interfaces on polymerized/solvate ionic liquids
- Studied the transition of electrical double layer from ionic liquid to aqueous solution near charged nanorods
- Analyzed the electrostatic effects on structural forces between nanorods
- Elucidated the effects of surface ionization on water transport and salt leakage through graphene oxide membranes

Oak Ridge National Laboratory, Oak Ridge, TN

6/2017 – 8/2017

Visiting Student

- Examined the effects of structural distortion on the reduction of Li⁺ ions in solvate ionic liquid using DFT along with natural bond orbital calculations

Shandong University, Jinan, China

8/2012 – 6/2015

Research Assistant

- Designed a dynamic cyclone on gas-solid separation used in coal-fired power plants
- Optimized the structure and dimension of the dynamic cyclone using experiments and simulations

JOURNAL PUBLICATIONS

Peer Reviewed Journal Papers (Publications are summarized in [Google Scholar](#) with >40 papers and > 800 citations. *equal contribution, [representative papers in blue](#));

- (1) [Yu, Z.*](#); [Shi, Z.*](#); [Bheemireddy, S. R.](#); [Kamphause, E.](#); [An, B.](#); [Uddin, M. A.](#); [Li, Z.](#); [Yang, Z.](#); [Xu, K.](#); [Li, T.](#); [Moore, J. S.](#); [Zhang, L.](#); [Cheng, L.](#); [Simulation Guided Molecular Design of Hydrofluoroether Solvent for High Energy Batteries, *ACS Energy Letter* **2022**. \(submitted\)](#)
- (2) [Mistry, A.](#); [Yu, Z.](#); [Cheng, L.](#); [Srinivasan, V.](#); [On Relative Importance of Correlated and Uncorrelated Molecular Motions in Defining Electrolyte Transport, *ACS Central Science* **2022**. \(submitted\)](#)

- (3) Mistry, A.; **Yu, Z.**; Peters, B. L.; Fang, C.; Wang, R.; Curtiss, L. A.; Balsara, N. P.; Cheng, L.; Srinivasan, V.; Toward Bottom-up Understanding of Transport in Concentrated Battery electrolytes, *ACS Central Science* **2022**, *8*, 880–890.
- (4) Yang, J.; Rodrigues, M. T.; **Yu, Z.**; Son, S. B.; Liu, K.; Dietz Rago, N. L.; Cheng, L.; Zhang, Z.; Liao, C., Design of a Scavenging Pyrrole Additive for High Voltage Lithium Ion Batteries. *Journal of the Electrochemical Society* **2022**, *169*, 040507
- (5) Peters, B. L.; **Yu, Z.**; Redfern, P. C.; Curtiss, L. A.; Cheng, L., Effects of Salt Aggregation in Perfluoroether Electrolytes. *Journal of the Electrochemical Society* **2022**, *169*, 020506
- (6) **Yu, Z.**; Balsara, N. P.; Borodin, O.; Gewirth, A. A.; Hahn, N. T.; Maginn, E. J.; Persson, K.; Srinivasan, V.; Toney, M. F.; Xu, K.; Zavadil, K.; Curtiss, L. A.; Cheng, L., Beyond Local Solvation Structure: Nanometric Aggregates in Battery Electrolytes and their Effect on Electrolyte Properties. *ACS Energy Letters* **2022**, *7*, 461-470.
- (7) Qian, K.*; **Yu, Z.***; Liu, Y.; Gosztola, D. J.; Winans, R. E.; Cheng, L.; Li, T., Understanding Fluorine-Free Electrolytes via Small-Angle X-Ray Scattering. *Journal of Energy Chemistry* **2022**, *70*, 340-346.
- (8) **Yu, Z.**; Juran, T. R.; Liu, X.; Han, K. S.; Wang, H.; Mueller, K. T.; Li, T.; Curtiss, L. A.; Cheng, L., Solvation Structure and Dynamics of Mg(TFSI)₂ Aqueous Electrolyte. *Energy & Environmental Materials* **2022**, *5*, 295-304.
- (9) Wen, X.; **Yu, Z.**; Zhao, Y.; Zhang, J.; Qiao, R.; Cheng, L.; Ban, C.; Guo, J., Enabling Magnesium Anodes by Tuning the Electrode/Electrolyte Interfacial Structure. *ACS Applied Materials & Interfaces* **2021**, *13*, 52461-52468.
- (10) Zhao, Y.; Zhang, J.; Agarwal, G.; **Yu, Z.**; Corman R. E.; Wang, Y.; Robertson, L. A.; Shi, Z.; Doan, H. A.; Ewoldt, R. H.; Shkrob, I. A.; Assary, R. S.; Cheng, L.; Srinivasan, V.; Babinec, S. J.; Zhang, L., TEMPO Allegro: Liquid Catholyte Redoxmers for Nonaqueous Redox Flow Batteries. *Journal of Materials Chemistry A* **2021**, *9*, 16769-16775.
- (11) Shkrob, I. A.; Robertson, L. A.; **Yu, Z.**; Assary, R. S.; Cheng, L.; Zhang, L.; Sarnello, E.; Liu, X.; Li, T.; Kaur, A. P.; Suduwella, T. M.; Odom, S. A.; Wang, Y.; Ewoldt, R. H.; Farag, H.; Zhang, Y., Crowded Electrolytes Containing Redoxmers in Different States of Charge: Solution Structure, Properties, and Fundamental Limits on Energy Density. *Journal of Molecular Liquids* **2021**, *334*, 116533.
- (12) Su, C.-C.; He, M.; Shi, J.; Amine, R.; **Yu, Z.**; Cheng, L.; Guo, J.; Amine, K., Principle in Developing Novel Fluorinated Sulfone Electrolyte for High Voltage Lithium-ion Batteries. *Energy & Environmental Science* **2021**, *14*, 3029-3034.
- (13) Su, C.-C.; He, M.; Amine, R.; Chen, Z.; **Yu, Z.**; Rojas, T.; Cheng, L.; Ngo, A. T., Unveiling Decaying Mechanism through Quantitative Structure-Activity Relationship in Electrolytes for Lithium-ion Batteries. *Nano Energy* **2021**, *83*, 105843.
- (14) Liu, X.; Daali, A.; Zhou, X.; **Yu, Z.**; Li, X.; Liu, Y.; Yin, L.; Yang, Z.; Zhao, C.; Zhu, L.; Ren, Y.; Shan, N.; Cheng, L.; Chen, Z.; Xu, G.-L.; Amine, K., Stress- and Interface-Compatible Red Phosphorus Anode for High-Energy and Durable Sodium-Ion Batteries. *ACS Energy Letters*. **2021**, *6*, 547-556.
- (15) Liu, X.; **Yu, Z.**; Sarnello, E.; Qian, K.; Seifert, S.; Winans, R. E.; Cheng, L.; Li, T., Microscopic Understanding of the Ionic Networks of “Water-in-Salt” Electrolytes. *Energy Material Advances* **2021**, Article ID 7368420, 9 pages.

- (16) Zhao, C.; Xu, G.-L.; **Yu, Z.**; Zhang, L.; Huang, I.; Mo, Y.-X.; Ren, Y.; Cheng, L.; Sun, C.-J.; Ren, Y.; Zuo, X.; Li, J.-T.; Sun, S.-G.; Amine, K.; Zhao, T., A High-Energy and Long-Cycling Lithium-Sulfur Pouch Cell via a Macroporous Catalytic Cathode with Double-End Binding Sites. *Nature Nanotechnology* **2021**, *16*, 166-173.
- (17) Zhao, Y.*; **Yu, Z.***; Robertson, L. A.; Zhang, J.; Shi, Z.; Bheemireddy, S. R.; Shkrob, I. A.; Li, T.; Zhang, Z.; Cheng, L.; Zhang, L., Unexpected Electrochemical Behavior of an Anolyte Redoxmer in Flow Battery Electrolytes: Solvating Cations Help to Fight against the Thermodynamic–Kinetic Dilemma. *Journal of Materials Chemistry A* **2020**, *8*, 13470-13479.
- (18) Shkrob, I. A.; Li, T.; Sarnello, E.; Robertson, L. A.; Zhao, Y.; Farag, H.; **Yu, Z.**; Zhang, J.; Bheemireddy, S. R.; Zhang, Y.; Assary, R. S.; Ewoldt, R. H.; Cheng, L.; Zhang, L., Self-Assembled Solute Networks in Crowded Electrolyte Solutions and Nanoconfinement of Charged Redoxmer Molecules. *The Journal of Physical Chemistry B* **2020**, *124*, 10226-10236.
- (19) **Yu, Z.**; Curtiss, L. A.; Winans, R. E.; Zhang, Y.; Li, T.; Cheng, L., Asymmetric Composition of Ionic Aggregates and the Origin of High Correlated Transference Number in Water-in-Salt Electrolytes. *The Journal of Physical Chemistry Letters* **2020**, *11*, 1276-1281.
- (20) Zhao, Y.; Sarnello, E.; Robertson, L. A.; Zhang, J.; Shi, Z.; **Yu, Z.**; Bheemireddy, S. R.; Zhang, Y.; Li, T.; Assary, R. S.; Cheng, L.; Zhang, Z.; Zhang, L.; Shkrob, I. A., Competitive Pi-Stacking and H-bond Piling Increase Solubility of Heterocyclic Redoxmers in Flow Batteries. *The Journal of Physical Chemistry B* **2020**, *124*, 10409-10418.
- (21) Robertson, L. A.; Shkrob, I. A.; Agarwal, G.; Zhao, Y.; **Yu, Z.**; Assary, R. S.; Cheng, L.; Moore, J. S.; Zhang, L., Fluorescence-Enabled Self-Reporting for Redox Flow Batteries. *ACS Energy Letters* **2020**, *5*, 3062-3068.
- (22) Hahn, N. T.; Driscoll, D. M.; **Yu, Z.**; Sterbinsky, G. E.; Cheng, L.; Balasubramanian, M.; Zavadil, K. R., The Influence of Ether Solvent and Anion Coordination on Electrochemical Behavior in Calcium Battery Electrolytes. *ACS Applied Energy Materials* **2020**, *3*, 8337-8447.
- (23) Yang, M.; Leon, N.; Pan, B.; **Yu, Z.**; Cheng, L.; Liao, C., Mechanistic Insights in Quinone-Based Zinc Batteries with Nonaqueous Electrolytes. *Journal of the Electrochemical Society* **2020**, *167*, 100536.
- (24) Wang, Y.; Kaur, A. P.; Attanayake, N. H.; **Yu, Z.**; Suduwella, T. M.; Cheng, L.; Odom, S. A.; Ewoldt, R. H., Viscous Flow Properties and Hydrodynamic Diameter of Phenothiazine-Based Redox-Active Molecules in Different Supporting Salt Environments. *Physics of Fluids* **2020**, *32*, 083108.
- (25) Liu, K.; Jiang, S.; Dzwiniel, T.; Kim, H.; **Yu, Z.**; Dietz Rago, N. L.; Kim, J. J.; Fister, T. T.; Yang, J.; Liu, Q.; Gilbert, J. A.; Cheng, L.; Srinivasan, V.; Zhang, Z.; Liao, C., Molecular Design of a Highly Stable Single-Ion Conducting Polymer Gel Electrolyte. *ACS Applied Materials & Interfaces* **2020**, *12*, 29162-29172.
- (26) Lee, B. J.; Kang, T. H.; Lee, H. Y.; Samdani, J. S.; Jung, Y.; Zhang, C.; **Yu, Z.**; Xu, G. L.; Cheng, L.; Byun, S.; Lee, Y. M.; Amine, K.; Yu, J.-S., Revisiting the Role of Conductivity and Polarity of Host Materials for Long-Life Lithium-Sulfur Battery. *Advanced Energy Materials* **2020**, *10*, 1903934.
- (27) Han, K. S.; **Yu, Z.**; Wang, H.; Redfern, P. C.; Ma, L.; Cheng, L.; Chen, Y.; Hu, J. Z.; Curtiss, L. A.; Xu, K.; Murugesan, V.; Mueller, K. T., Origin of Unusual Acidity and Li⁺ Diffusivity in a Series of Water-in-Salt Electrolytes. *The Journal of Physical Chemistry B* **2020**, *124*, 5284-5291.

- (28) Wang, Y.; He, Y.; **Yu, Z.**; Gao, J.; Ten Brinck, S.; Slobodnick, C.; Fahs, G. B.; Zanelotti, C. J.; Hegde, M.; Moore, R. B.; Ensing, B.; Dingemans, T. J.; Qiao, R.; Madsen, L. A., Double Helical Conformation and Extreme Rigidity in a Rodlike Polyelectrolyte. *Nature Communications* **2019**, *10*, 1-8.
- (29) Jiang, Z.-L.; Xu, G.-L.; **Yu, Z.**; Zhou, T.-H.; Shi, W.-K.; Luo, C.-S.; Zhou, H.-J.; Chen, L.-B.; Sheng, W.-J.; Zhou, M.; Cheng, L.; Assary, R. S.; Sun, S.-G.; Amine, K.; Sun, H., High Rate and Long Cycle Life in Li-O₂ Batteries with Highly Efficient Catalytic Cathode Configured with Co₃O₄ Nanoflower. *Nano Energy* **2019**, *64*, 103896.
- (30) Jia, T.; Wang, Y.; Dou, Y.; Li, Y.; Jung de Andrade, M.; Wang, R.; Fang, S.; Li, J.; **Yu, Z.**; Qiao, R.; Liu, Z.; Cheng, Y.; Su, Y.; Minary-Jolandan, M.; Baughman, R. H.; Qian, D.; Liu, Z., Moisture Sensitive Smart Yarns and Textiles from Self-Balanced Silk Fiber Muscles. *Advanced Functional Materials* **2019**, *29*, 1808241.
- (31) **Yu, Z.**; Yang, F.; Dai, S.; Qiao, R., Structure and Dynamics of Polymeric Canopies in Nanoscale Ionic Materials: An Electrical Double Layer Perspective. *Scientific Reports* **2018**, *8*, 1-11.
- (32) **Yu, Z.**; Fang, C.; Huang, J.; Sumpter, B. G.; Qiao, R., Solvate Ionic Liquids at Electrified Interfaces. *ACS Applied Materials & Interfaces* **2018**, *10*, 32151-32161.
- (33) **Yu, Z.**; Fang, C.; Huang, J.; Sumpter, B. G.; Qiao, R., Molecular Structure and Dynamics of Interfacial Polymerized Ionic Liquids. *The Journal of Physical Chemistry C* **2018**, *122*, 22494-22503.
- (34) Zhang, F.; **Yu, Z.**; Rondinone, A. J.; Huang, J.; Sumpter, B. G.; Qiao, R., Adsorption of Molecular Nitrogen in Electrical Double Layers near Planar and Atomically Sharp Electrodes. *Langmuir* **2018**, *34*, 14552-14561.
- (35) **Yu, Z.**; Zhang, F.; Huang, J.; Sumpter, B. G.; Qiao, R., Ionic Liquids-Mediated Interactions between Nanorods. *The Journal of Chemical Physics* **2017**, *147*, 134704.
- (36) **Yu, Z.**; Wu, H.; Qiao, R., Electrical Double Layers near Charged Nanorods in Mixture Electrolytes. *The Journal of Physical Chemistry C* **2017**, *121*, 9454-9461.
- (37) Fang, C.; **Yu, Z.**; Qiao, R., Impact of Surface Ionization on Water Transport and Salt Leakage through Graphene Oxide Membranes. *The Journal of Physical Chemistry C* **2017**, *121*, 13412-13420.
- (38) **Yu, Z.**; He, Y.; Wang, Y.; Madsen, L. A.; Qiao, R., Molecular Structure and Dynamics of Ionic Liquids in a Rigid-Rod Polyanion-Based Ion Gel. *Langmuir* **2017**, *33*, 322-331.
- (39) **Yu, Z.**; Zhao, M.; Ma, C., Experimental and Numerical Investigations of a Dynamic Cyclone. *Proceedings of the Institution of Mechanical Engineers, Part A: Journal of Power and Energy* **2014**, *228*, 536-549.
- (40) **Yu, Z.**; Ma, C., Theoretical and Experimental Investigations on Separation Efficiency of a Dynamic Cyclone. *Modern Chemical Industry (Chinese)* **2014**, *34*, 122-125.
- (41) **Yu, Z.**; Ma, C., Numerical and Experimental Investigations of a Dynamic Cyclone. *Chemical Industry and Engineering Progress (Chinese)* **2014**, *33*, 1684-1690.

Book Chapter

- (1) **Yu, Z.**; Qiao, R., "Ionic Liquids in Molecular Composites" in "Encyclopedia of Ionic Liquids", edited by Suojiang Zhang, Elsevier, 2020.

SELECTED PRESENTATIONS AND POSTERS

1. Molecular structure of solvate ionic liquid at electrified interfaces, Oak Ridge National Laboratory, Oak Ridge, TN, 7/2017
2. Structure and dynamics of solid-like ion gels with high ionic conductivity, ACS Fall Meeting, Washington, DC, 8/2017
3. Ionic liquids-mediated interactions between nanorods, CSB Symposium, Blacksburg, VA, 5/2018
4. Structure and dynamics of polymeric canopies in nanoscale ionic materials: an electrical double layer perspective, CSB Symposium, Blacksburg, VA, 5/2018
5. Molecular dynamics simulation primer on polymer electrolytes, Shandong University, Jinan, China, 7/2018
6. Molecular dynamics simulation on novel polymer electrolytes, Huazhong University of Science and Technology, Wuhan, China, 7/2018
7. Molecular properties of advanced electrolytes featuring ionic liquids at electrified interfaces, Argonne National Laboratory, Lemont, IL, 9/2018
8. Solvation structure and dynamics of Mg(TFSI)₂ aqueous electrolyte, ACS Fall Meeting, San Diego, CA, 8/2019
9. Molecular properties of advanced electrolytes using multiscale simulations, Los Alamos National Laboratory, Los alamos, NM, 5/2021 (Online)
10. Molecular designing and characterizing of fluorinated ether solvents for Li metal batteries, ACS Fall Meeting, Atlanta, GA, 8/2021 (Online)
11. Physicochemical properties of advanced electrolytes using molecular simulations, University of Arkansas, Fayetteville, AR, 3/2022

MENTORING/TEACHING/OUTREACH EXPERIENCES

Mentoring

- Mentored a visiting graduate student, Taylor Juran, from Binghamton University on the solvation structure of multivalent ion in liquid electrolytes project, Argonne National Lab, 6/2019~8/2019.
- Mentored a graduate student, Xinyi Liu, from Northern Illinois University on the solvation transition in water-in-salt electrolytes project, Argonne National Lab, 2/2020~8/2020.

Teaching

- Delivered lectures on “Solvation, Structural, and Hydration Forces” for an internal summer course, Virginia Tech, 7/2017.
- Served as a teaching assistant for the undergraduate class of “Emissions and Control of Coal-Fired Pollutants”, Shandong University, 2/2014~6/2014.

Outreach

- Served as a volunteer for the 2018 Virginia Tech Science Festival, Virginia Tech, 10/2018.
- Delivered lectures to German graduate students at the China-Germany University Communication, Shandong University, 9/2013.

INDUSTRIAL EXPERIENCES

- | | |
|---|----------------|
| Chalu Street Thermal Power Plant , Jinan, China | 1/2014-5/2014 |
| • Measured dust removal efficiency of wet electrostatic precipitators | |
| Chun Yuan Air Blower Factory , Weifang, China | 11/2013-4/2014 |
| • Gauged flow rate and pressure drop of air blowers | |
| China Guodian Corporation Yiyang Power Plant , Yiyang, China | 5/2013-6/2013 |
| • Measured dust removal efficiency of wet electrostatic precipitators | |
| China Huaneng Group Laiwu Power Plant , Laiwu, China | 5/2011-6/2011 |
| Conducted professional internships in power plant operation | |

SUPERCOMPUTER TIME GRANTS

1. PI, Project: Ionic Liquids for Rare Earth Elements Separations, 2,000,000 GPU Hours, Los Alamos National Laboratory Institutional Computing program, 2022
2. PI, Project: Solvation to Electrolyte Properties, 700,000 CPU Hours, Argonne National Laboratory Computing Resource Center, 2019
3. PI, Project: Physicochemical Properties of Multivalent Electrolytes, 700,000 CPU Hours, Argonne National Laboratory Computing Resource Center, 2019

AWARDS/ACCOMPLISHMENTS

1. Joint Center for Energy Storage Research (JCESR) Publications Awards, as the first author on the publication "Beyond Local Solvation Structure: Nanometric Aggregates in Battery Electrolytes and their Effect on Electrolyte Properties", 2022 – Awarded to 5 recipients each year from a pool of ~100 publications in JCESR
2. China National Scholarship, 2015 – Highest honor for graduate students in China (2:1000 award rate)
3. Jing Cheng Shu Kong Scholarship, 2014 – Awarded to 10 master students every year from an application pool of ~600 master students in Shandong University

TECHNICAL SKILLS

Programming: C, Matlab, Perl, Bash

Simulation packages: GROMACS, LAMMPS, CP2K, Gaussian, VASP, ANSYS, COMSOL

Visualization: VMD, Tecplot, Gnuplot, Grace

Operating systems: macOS, Linux, Microsoft Windows

REVIEWER SERVICE & PROFESSIONAL MEMBERSHIPS

Referee for Peer-Reviewed Journals:

- The Journal of Physical Chemistry C
- Langmuir

- Chemical Physics Letters
- Physical Chemistry Chemical Physics
- Scientific Reports
- AIChE Journal
- Fuel
- Advances in Materials Science and Engineering
- International Journal of Heat and Mass Transfer
- International Communications in Heat and Mass Transfer
- Journal of Thermal Science and Engineering Applications
- Molecular Systems Design & Engineering
- Applied Surface Science
- Applied Sciences
- Symmetry
- Water

Professional Memberships

- ACS and APS