Communicating Science

Telling Your Story Through Poster Presentations

August 15, 2015

Presenters:

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Larisa Blyudaya, Independent Senior Graphic Designer

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Why Communication Matters?

Societal Impact

"Science is an enormous force behind the betterment of society"
— Martin Alcorta, Postdoctoral Alumni (PHY), 2013

Impact on Scientific Community

"There is so much going on in the HEP group at Argonne, barely a day goes by when I don't hear about something I find incredible"
—Lily Asquith, HEP Postdoctoral Appointee

Impact on Next Generation of STEM Professionals

"Not only do they [outreach events] have a genuine and lasting effect on the next generation of researchers, but they are also extremely fulfilling for mentors"
—Helena David, PHY Postdoctoral Appointee

Honing Your Own Skills

"I think that many of us postdocs say that we want to be teachers, but we have very little real teaching experience"
—Erin Iski, Postdoctoral Alumna (CNM), 2013

Read more at: https://blogs.anl.gov/postdoc/category/communicating-science/

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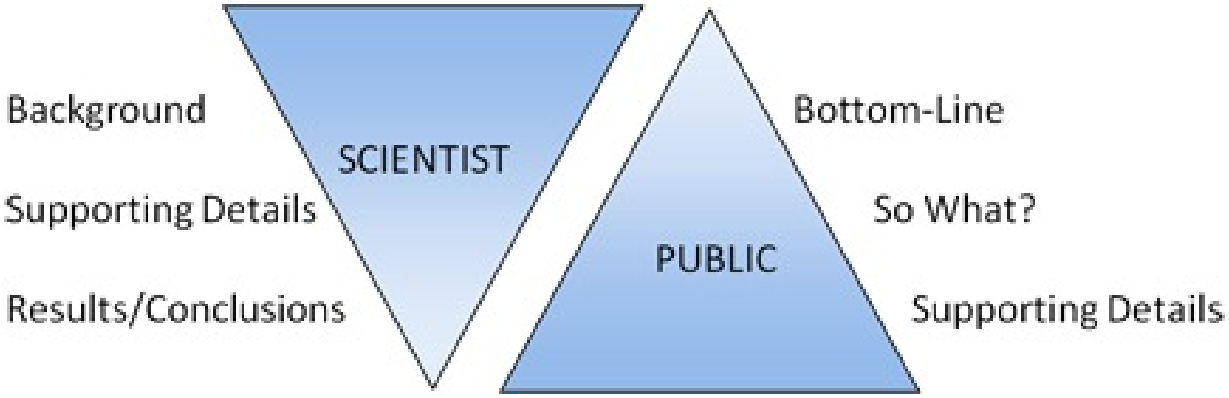
Communicating Science in Three (Sort of) Simple Steps

1. Know Your Audience
2. Define Three Major Points You'd Like to Communicate
3. Tell Your Story



Learn more at: http://www.aaas.org/communicatingscience

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Communicating Science in Three (Sort of) Simple Steps

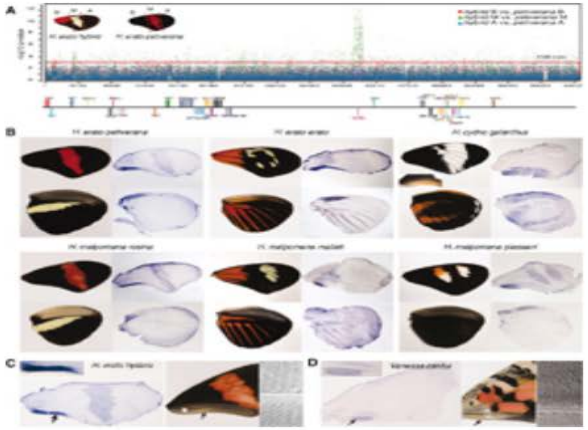
optix Drives the Repeated Convergent Evolution of Butterfly Wing Pattern Mimicry

(Reprinted from Reed et al., *Science* 333 (6046) 1137-1141.)

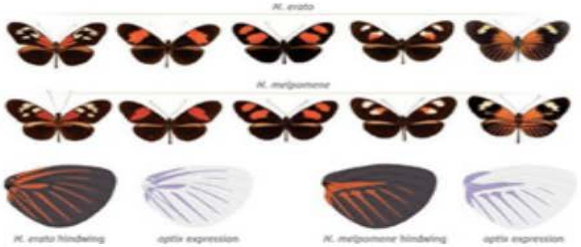
How Great Wings Can Look Alike

(Reprinted from Carroll, *Science* 333 (6046) 1100-1101.)

SPECIALIST



VS



GENERALIST

Learn more at: http://www.aaas.org/communicatingscience

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Purpose and Modes of Science Communication

Report research findings to a community:

- Scientific community
- Funding agencies
- Management
- General Public

Modes:

- Research Papers
- Popular press articles
- Oral presentations
- Poster presentations

Added bonus of allowing direct networking and discussion

Elements of a poster presentation

- Know audience—specialist vs. generalist?
- What do you want the audience to know?
- Can I still have interesting title for specialist audience, but avoid being too “cute”?
- Major elements—Introduction, Methods, Results, Conclusions, Acknowledgements, References
- How do people find you?—Include contact information at the end.
- Don’t be too wordy—Purrington recommends ~500 words.

Remember — It’s a story!

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Standard Poster Judging Criteria

Overall Poster Appearance
(Would someone walking past this poster be motivated to stop and read it? Does this poster grab your attention?)

Topic Organization
(Easy to follow, organization draws you through the poster)

Presenters Ability to Adequately Answer Questions
(Presenter shows good command of topic, answers all questions in a professional and concise manner)

Overall Presentation Quality
(Presenters ability to explain work and results clearly and concisely)

Clarity/Significance of Illustrations
(Do illustrations used clearly convey significant information? Is there a better way to illustrate the information?)

Overall Poster Quality

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Poster Abstracts Are All About What?

- Short, concise, but flows nicely.
- What are you doing?
- Why is it important?—AKA, Who Cares?
- What did you find?
- What's next?
- Note: Poster does not typically have the abstract on it—this is usually included in a conference abstract book

Anaeromyxobacter dehalogenans 2CP-C is a delta-Proteobacteria that thrives on a wide range of substrates, including chlorinated phenolic compounds, nitrate, fumarate, iron oxyhydroxides, and uranium. This metabolic versatility, together with its presence in contaminated subsurface sites, makes *Anaeromyxobacter* spp. attractive candidates for in situ bioremediation processes. Using 2-dimensional gel electrophoresis, we examined the global cell proteome of iron-exposed cells to reveal iron-responsive proteins in strain 2CP-C to gain insight into the metabolic response of this strain to environmentally-relevant growth conditions. A novel protein of unknown function (Adeh0974) exhibited a dramatic in expression in response to iron. Computational analysis showed Adeh0974 to be structurally similar to OmpF, an outer membrane protein involved in electron transfer. An investigation of the synteny of Adeh0974 revealed that this gene and a nearby cytochome c-type gene (Adeh0972) are well conserved across diverse proteobacterial groups, including known metal reducers. These findings indicate a potential role for Adeh0974 in electron transfer mechanisms, specifically in the response to iron. The putative Adeh0974-0972 operon is being investigated at the transcript level for similar expression changes.

Why? Who Cares?

What am I doing?

What did I find?

What's Next?

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Writing an Abstract (Step-by-Step Process)

1. Write **1-2 introduction sentences** that explain topic, purpose, and research question(s).
2. Write **1-2 sentences describing** your research **methods** (this may also include the type of data analysis you used).
3. Write **1-2 sentences describing the results** / findings
4. Write **1-2 sentences** containing your **conclusions** and recommendations.

Reference: http://owl.english.purdue.edu/

Writer and Designer: Purdue OWL (Purdue Online Writing Lab) | Updated by H. Allen Brizee, 2007; Arielle McKee, 2014
Developed with resources courtesy of the Purdue University Writing Lab |

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Introduction

Key Elements

- What are you doing?
- Why is it important?
- Not a repeat of your abstract!
- If pictures and diagrams are helpful, use them.

Introduction

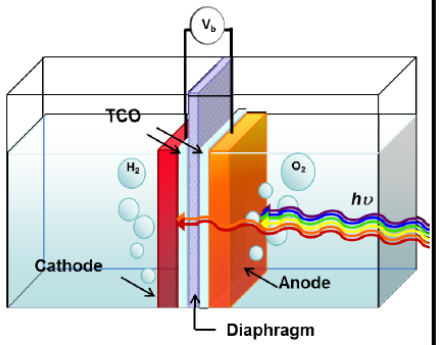
Deep water coral reefs (30-100m) could shelter commercial fish stocks and provide coral larvae for recovering shallow reefs. Deep corals appear healthier than shallow corals, but depth has restricted their study. Current quantitative study methods involve scattering random points across images and visually identifying substrates.

Montastrea annularis complex is a major reef building coral representing as much as 75% of the coral cover in some areas. Its dominance and smooth texture make it an ideal candidate for image processing. The goal of this research was to develop an algorithm to segment out colonies of the *M. annularis* complex and calculate percent coverage values.

Source: http://www.writing.engr.psu.edu/samples/poster7.pdf

Background

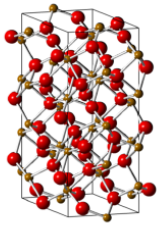
- The conversion of solar energy to chemical energy via photoelectrochemical (PEC) water splitting is a promising route to renewable fuel production.
- Efficient utilization of solar fuels mitigate the negative effects of carbon-based fuel sources.



Hematite (α-Fe_2O_3):

Advantages:
- Suitable band gap
- Earth-abundant
- Stable in aqueous
- Non-toxic

Disadvantages
- Deep $h\nu$ penetration
- Short h^+ diffusion
- High e^-/h^+ recombination
- Slow OER kinetics



$H_2O \rightarrow \frac{1}{2}O_2 + H_2$ $\Delta G = 1.23$ eV

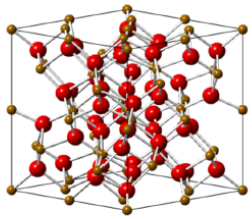
$2H_2O \rightarrow O_2 + 4H^+ + 4e^-$ (OER)

$2H^+ + 2e^- \rightarrow H_2$ (HER)

Alternate Phase (β-Fe_2O_3):
- Bixbyite crystal structure
- Elusive and metastable
- Unknown PEC properties
- Potential Advantages:
  - Smaller band gap
    - Improved long-λ photoconversion
    - Increased overall efficiency
    - Ideal for tandem absorber cells
  - Differing surface structure
    - Improved OER kinetics
    - Improved catalytic reactivity

Differing bulk properties
- Improved charge transport
- Increase absorption

Isomorphic with ITO
- Epitaxy
- Directed crystal growth
- Control of surface truncation
- Improved crystallinity



Further information

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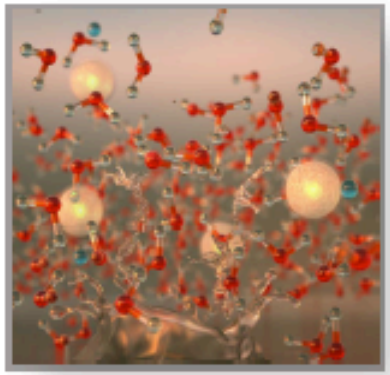
Introduction

Introduction

Knowledge of the structure of water and solutions of salts is important both from fundamental standpoint and for describing many systems and processes of practical significance:



More accurate description of **biologically significant molecules** in solutions of salts (saline)

Systems with interfaces:
- Materials for photocatalytic water splitting;
- Properties of atmospheric aerosols

Despite extensive research, many properties of water and solutions of salts are not completely understood, e.g.

Do dissolved salts have long-range effect on the structure of water, or is their effect limited to the first solvation shell of ions?

Reason: Experiments cannot probe the structure of hydrogen-bonded liquids directly, they provide only indirect information about the average structure of water and solutions

Simulations, especially from first principles, complement experimental measurements of the structure of water and solutions of salts, and can be used to interpret and validate experiments

Methods

Key Elements

- What did you do?
- Not an exhaustive list of every. Little. Thing. You. Did.
- Brief summary of what you did.
- Flow chart, graphics may be useful to minimize text.

I prepared bicarbona buffer mineral media by first adding minerals X, water. Then I added the carbon source to solution. Then I adjusted the pH to 6.5 meter and bicarbonate buffer the solution by….

- Bacteria were grown anaerobically in bicarbonate-buffered mineral media with acetate as the electron donor and harvested after 48 hours.
- Whole cell extract proteins were prepared by sonication of cell pellets and separated by two-dimensional gel electrophoresis (2DGE).
- Statistically-significant differences in relative protein abundance between growth conditions were determined based on the integrated density of silver-stained protein spots.
- Proteins were identified by tandem mass spectrometry of tryptic digests.

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Results

Key Elements

What did you find?

Include the most important results of your research—what really helped you answer your question?

What's the best way to present your data?

- Graphs?
- Table?
- Image?

Title and captions!

Arrange the way you want the viewer to read.

Results

Blah, blah, blah

Comparison of 2DGE Protein Profiles

Figure 1: Representative protein profiles of *Anaeromyxobacter dehalogenans* strain 2CP-C grown under nitrate and lepidocrocite exposure. Red circle indicates region surrounding Adeh_0974. Proteins that exhibited an increased abundance under lepidocrocite exposure were identified by LC-MS/MS (Tables 1-2).

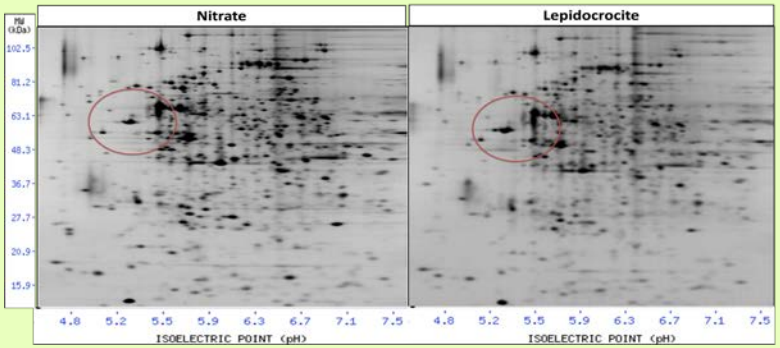


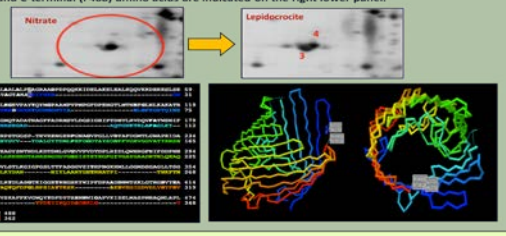
Table 1: Mass spectrometric identifications of putative membrane or transport proteins with increased abundance under lepidocrocite exposure versus the nitrate control condition.

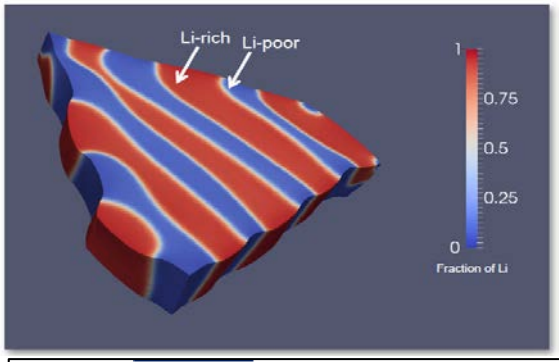
Adeh_0974 and Adeh_2423 annotated as "Hypothetical Proteins." Structure-based comparisons predict that these two are similar to OmpF porin proteins.

Locus	MW (kDa)	pI	Annotation
Adeh_0427	48.2	5.61	Outer Membrane Efflux Protein (TolC-like)
Adeh_0484	75	6.00	TonB-dependent receptor
Adeh_0622	62.6	5.13	Type II Secretion system protein E
Adeh_0974	52.9	5.42	Protein of Unknown Function; Putative OmpF-type Protein
Adeh_2423	45.5	8.71	Protein of Unknown Function; Putative OmpF-type Protein
Adeh_3337	25.7	5.28	OmpA/MotB Family Outer Membrane Protein
Adeh_3747	57	5.73	OmpA/MotB Family Outer Membrane Protein

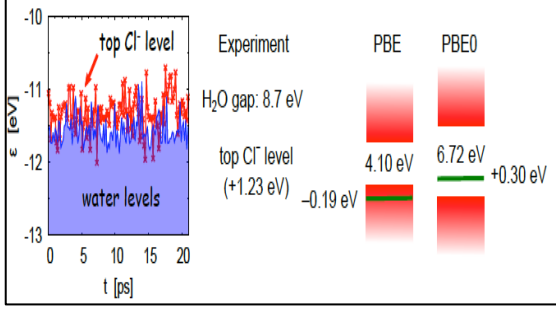
A Closer Look at Adeh_0974

Figure 2: Increased abundance of Adeh_0974 (spot 3) under Lepidocrocite conditions (right top panel) versus Nitrate conditions (left top panel). Annotated as a Hypothetical Protein, Adeh_0974 has an N-terminal signal recognition sequence. Sequence comparisons yielded no hits to functionally characterized proteins. Structure-based comparisons using PSI-BLAST and Fold & Function Assignment System 3.0 (www.ffas.burnham.org) strongly suggest that Adeh_0974 is a Beta-barrel membrane porin of the OmpF family. Sequence alignment of Adeh_0974 and OmpF (*E. coli*) and predicted structure of Adeh_0974 are shown in the bottom panel. The N-terminal (L21) and C-terminal (F488) amino acids are indicated on the right lower panel.





We performed this analysis for NaCl solutions using PBE and PBE0 functionals:



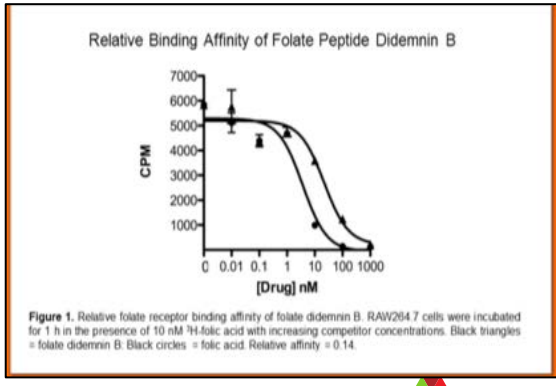


Figure 1. Relative folate receptor binding affinity of folate didemnin B. RAW264.7 cells were incubated for 1 h in the presence of 10 nM ^{3}H-folic acid with increasing competitor concentrations. Black triangles = folate didemnin B; Black circles = folic acid. Relative affinity = 0.14.

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Conclusions

Key Elements

Often read first!

Not a repeat of your results.

What did you conclude from the results?

How does this conclusion fit with what others have found?

What is known in the literature?

What should be done next?

Conclusions

- A thiol conjugatable form of didemnin B was synthesized.
- Coupling of the didemnin B construct to a folate cysteinyl peptide afforded a releasable, water soluble prodrug.
- The prodrug demonstrated excellent binding affinity, cytotoxicity, and TNF-α inhibition in RAW264.7 cells. TNF-α inhibition appeared to mirror cytotoxicity.
- Future studies will be undertaken to assess whether there is comparable activity in activated peritoneal macrophages.

4. CONCLUSIONS AND FINAL REMARKS

The submicron fraction (<0.7 μm) had mostly a lower contribution to the bulk b_{bp} (33±8%), but a strong linear relation with Chl*a*, as well as HB and the PSD slope (<3 μm). This suggests that smaller particles e.g., submicron detritus, virus and HB, may not be as strong b_{bp} contributors as predicted by Mie theory, but they are likely the main sources regulating the b_{bp} relation with Chl*a* and PSD. This may be explained by a tight relation between the concentration of these small and rather roundish particles with the trophic state indexed by Chl*a*. Larger phytoplankton sized particles are likely stronger b_{bp} contributors due to their complex structures and/or presence of high index particles, but they introduce a greater dispersion in the Chl*a* relation, instead of relating directly the carbon content to b_{bp}. The results have implications for ocean color modeling and highlight the importance of further *in situ* and modeling experiments to properly describe the sources of marine b_{bp}.

Above source: http://www.eposters.net/poster/particle-backscattering-coefficient-and-its-relation-to-biogeochemical-properties-in-the-southern

Conclusions

Blah, blah, blah

Literature cited

Blah, blah, and blah. 2012. Blahing, blahing, and more blahing. *Journal of Blahology* 1:1-2.
Blah, blah, and blah. 2012. Blahing, blahing, and more blahing. *Journal of Blahology* 1:1-2.
Blah, blah, and blah. 2012. Blahing, blahing, and more blahing. *Journal of Blahology* 1:1-2.

Acknowledgments

Blah, blah, blah. This file from http://colinpurrington.com/tips/academic/posterdesign. You can erase that URL, of course.

Further information

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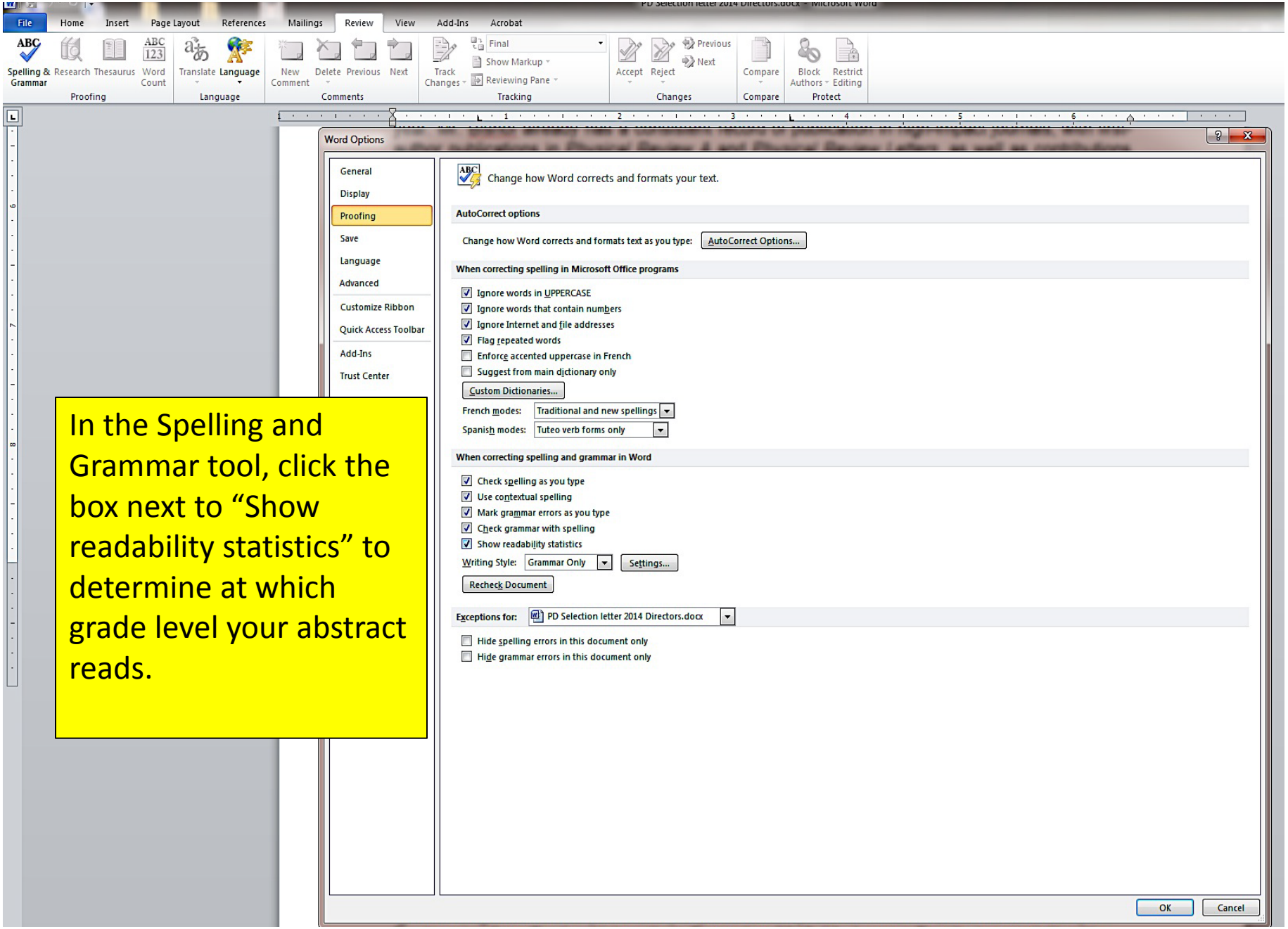
Am I Getting My Message Across?

Content:

- Language is appropriate for audience
- Data presented in proper format
- Word usage reflect “big picture”

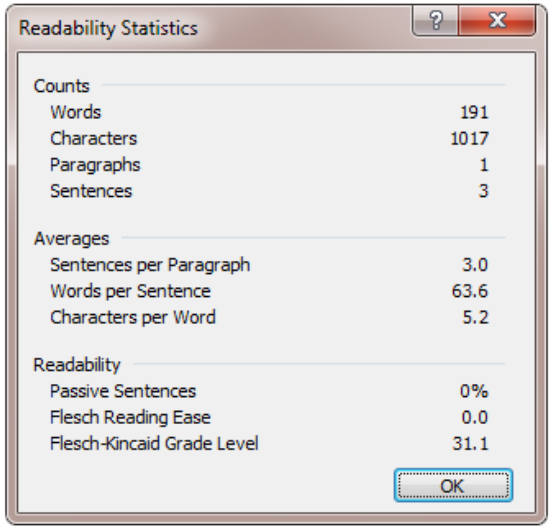
Tools:

- Microsoft Word
  “Readability Tool”
- Extremepresentation.typepad.com
  Chart chooser
- Visual-literacy.org
  Periodic Table of Visualization Methods—interactive map of chart types and examples of use
- Wordle.net
  Word Cloud



In the Spelling and Grammar tool, click the box next to “Show readability statistics” to determine at which grade level your abstract reads.

The supply of clean and sustainable energy is perhaps the most important scientific challenge facing society today . Currently the energy demand is predominantly met by fossil fuels which generate harmful greenhouse gases, Will the global energy demand expected to at least double by midcentury due to population and economic growth, renewable energy resources have become a major aspect of US energy research activities , Among renewable energy resources, solar energy is by far the largest usable resource, providing more energy in 1 hour to the earth than all of the energy consumed by humans in an entire year. Nature has found a way to utilize the sun's energy in the process of photosynthesis, in which sunlight and water are stored in the chemical bonds of oxygen and carbohydrates. We have developed a new approach that links Nature's inherent photosynthetic chemistry with a synthetic molecular catalyst or nanoparticle to create a hybrid complex that uses light to rapidly produce hydrogen directly from water .The goal of this work is to link an earth- abundant catalyst to cyanobacterial Pholosystem-1 (PSI) that will allow us to produce hydrogen in an affordable and environmentally clean manner.

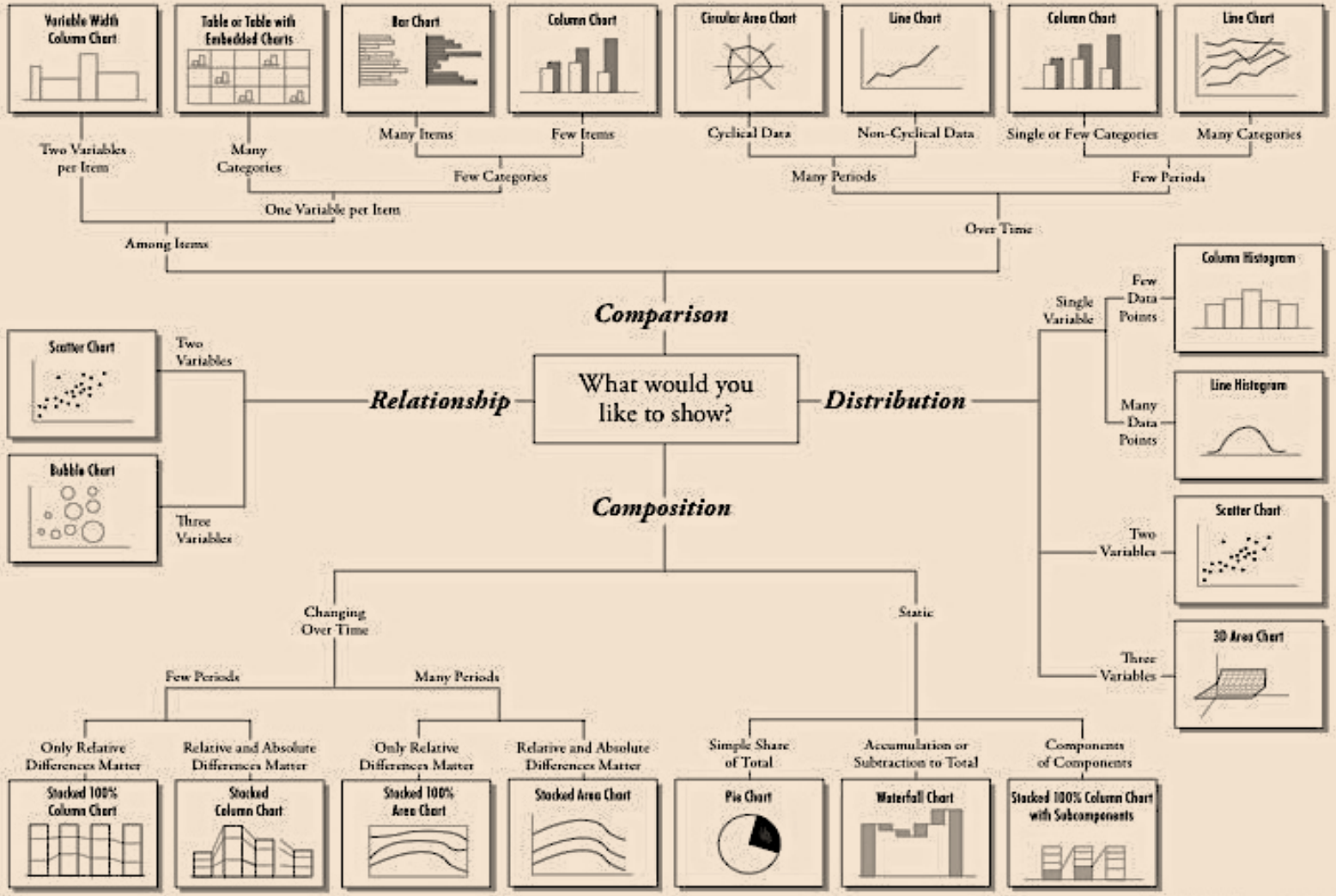


Newspapers aim for a reading level of grade 8.

This abstract reads at grade 31.1.

Might want to do a bit of editing!

Chart Suggestions—A Thought-Starter



A PERIODIC TABLE OF VISUALIZATION METHODS

Data Visualization
Visual representations of quantitative data in schematic form (either with or without axes)

Information Visualization
The use of interactive visual representations of data to amplify cognition. This means that the data is transformed into an image, it is mapped to screen space. The image can be changed by users as they proceed working with it

Concept Visualization
Methods to elaborate (mostly) qualitative concepts, ideas, plans, and analyses.

Strategy Visualization
The systematic use of complementary visual representations in the analysis, development, formulation, communication, and implementation of strategies in organizations.

Metaphor Visualization
Visual Metaphors position information graphically to organize and structure information. They also convey an insight about the represented information through the key characteristics of the metaphor that is employed

Compound Visualization
The complementary use of different graphic representation formats in one single schema or frame

>☼< C continuum																	☼ G graphic facilitation
>◎< Tb table	>☼< Ca cartesian coordinates											>☼< Me meeting trace	>☼< Mm metro map	☼ Tm temple	<☼> St story template	>☼< Tr tree	¤ Ct cartoon
>☼< Pi pie chart	>☼< L line chart											>☼< Co communication diagram	>☼< Fp flight plan	>☼< Cs concept sceleton	☼ Br bridge	>☼< Fu funnel	☼ Ri rich picture
>☼< B bar chart	>☼< Ac area chart	>☼< R radar chart cobweb	>◎< Pa parallel coordinates	>◎< Hy hyperbolic tree	>☼< Cy cycle diagram	>☼< T timeline	>☼< Ve venn diagram	<◎> Mi mindmap	<☼> Sq square of oppositions	>☼< Cc concentric circles	>☼< Ar argument slide	>◎< Sw swim lane diagram	>☼< Gc gantt chart	<◎> Pm perspectives diagram	>◎< D dilemma diagram	<☼> Pr parameter ruler	☼ Kn knowledge map
>☼< Hi histogram	>☼< Sc scatterplot	>☼< Sa sankey diagram	>◎< In information lense	>¤< E entity relationship diagram	>☼< Pt petri net	>◎< Fl flow chart	<☼> Cl clustering	>☼< Le layer chart	>◎< Py minto pyramid technique	>☼< Ce cause-effect chains	>☼< Tl toulmin map	>◎< Dt decision tree	>¤< Cp cpm critical path method	<☼> Cf concept fan	>◎< Co concept map	☼ Ic iceberg	☼ Lm learning map
>☼< Tk tukey box plot	>☼< Sp spectogram	>☼< Da data map	>◎< Tp treemap	>◎< Cn cone tree	>☼< Sy system dyn./ simulation	>◎< Df data flow diagram	<☼> Se semantic network	>◎< So soft system modeling	◎ Sn synergy map	<☼> Fo force field diagram	>¤< Ib ibis argumentation map	>☼< Pr process event chains	>☼< Pe pert chart	<◎> Ev evocative knowledge map	>◎< V Yee diagram	<☼> Hh heaven 'n' hell chart	◎ I informural

Cy Process Visualization

Hy Structure Visualization

☼ Overview

¤ Detail

◎ Detail **AND** Overview

< > Divergent thinking

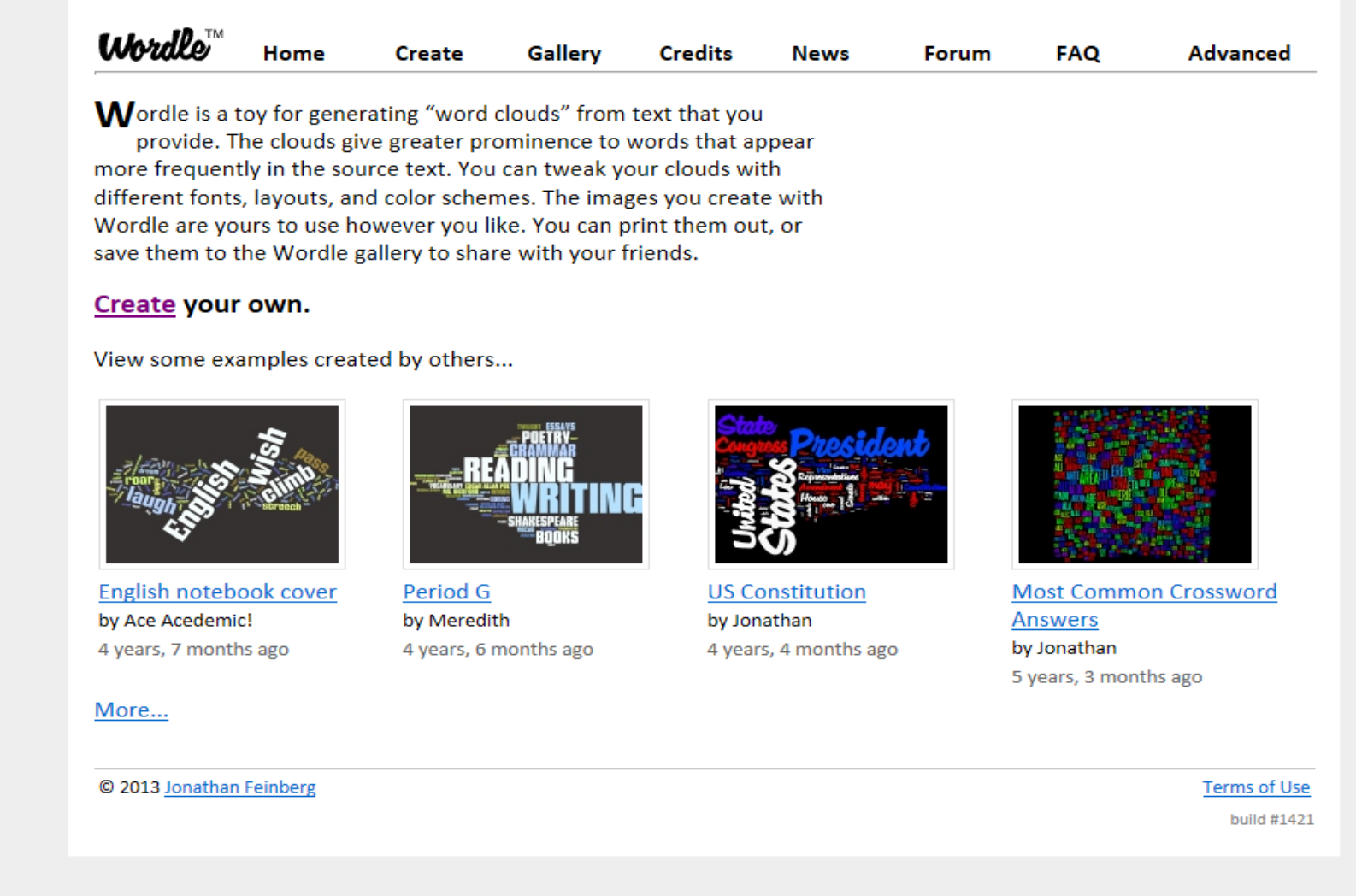
> < Convergent thinking

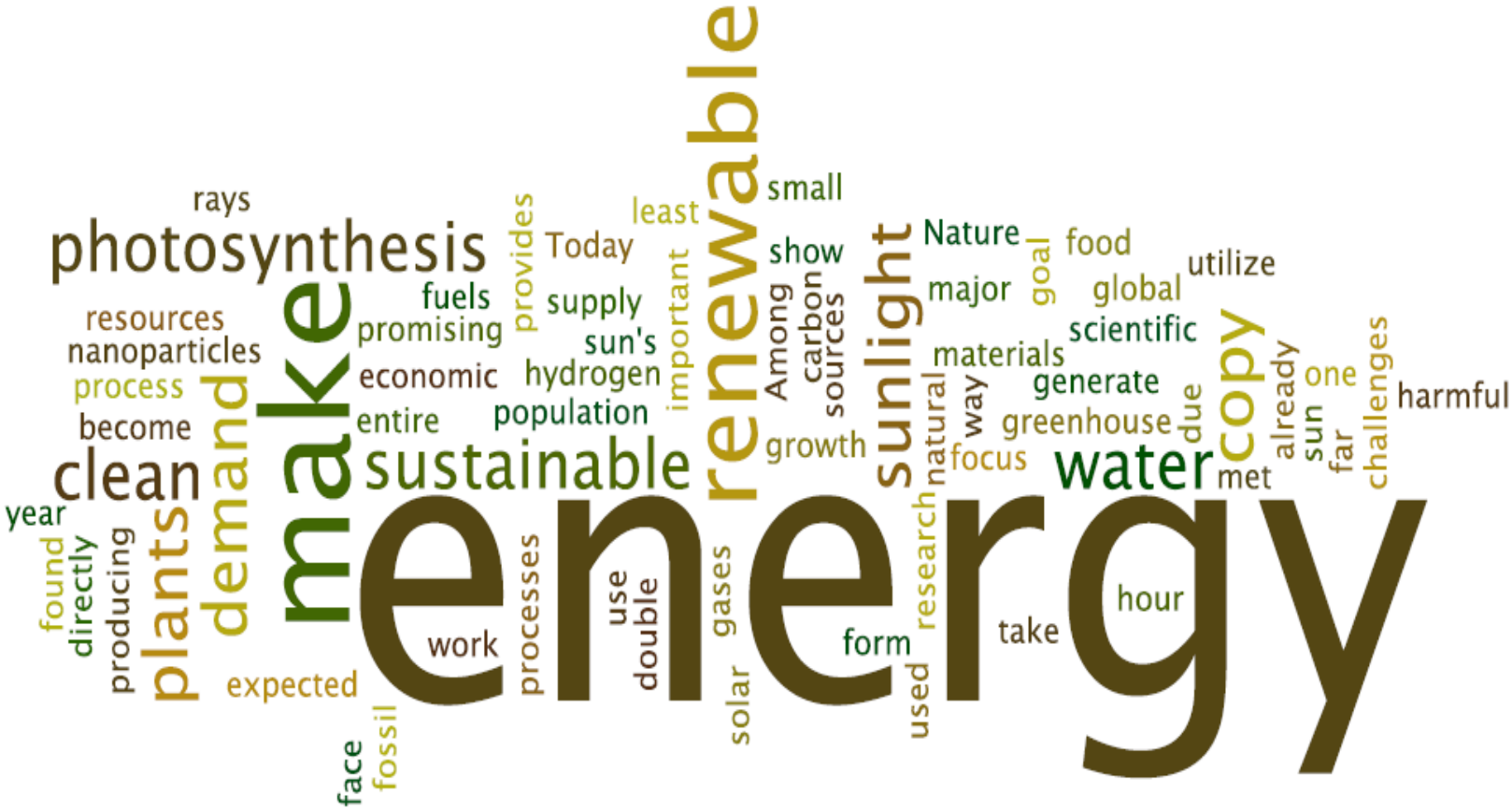
Note: Depending on your location and connection speed it can take some time to load a pop-up picture.

version 1.5

>☼< Su supply demand curve	>◎< Pc performance charting	>☼< St strategy map	>☼< Oc organisation chart	<¤> Ho house of quality	>☼< Fd feedback diagram	¤ Ft failure tree	>☼< Mq magic quadrant	>☼< Ld life-cycle diagram	>☼< Po porter's five forces	<¤> S s-cycle	>☼< Sm stakeholder map	◎ Is ishikawa diagram	☼ Tc technology roadmap
☼ Ed edgeworth box	>◎< Pf portfolio diagram	☼ Sg strategic game board	>☼< Mz mintzberg's organigraph	<¤> Z zwicky's morphological box	<◎> Ad affinity diagram	¤ De decision discovery diagram	>☼< Bm bcg matrix	>☼< Stc strategy canvas	>☼< Vc value chain	<¤> Hy hype-cycle	>☼< Sr stakeholder rating map	>☼< Ta taps	<¤> Sd spray diagram

Check word usage and make cool word clouds at www.wordle.net

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hydrogen
economic
entire
population
growth
processes
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used
form
take
hour

References

Highly Recommended:

- http://colinpurrington.com/tips/academic/posterdesign -- Poster guru
- http://www.ncsu.edu/project/posters/NewSite/-- Examples with critique
- https://docs.anl.gov/main/groups/intranet/@shared/@news/documents/publication/396002.pdf --CEPA tip sheet on creating successful scientific posters (Inside Argonne access only)
- http://betterposters.blogspot.com/ --Better Posters Blog with links to examples
- http://www.writing.engr.psu.edu/posters.html -- More examples
- http://extremepresentation.typepad.com
- http://www.visual-literacy.org/pages/documents.htm

How-To articles:

- http://www.nature.com/scitable/nated/topicpage/poster-presentations-13907939
- http://www2.napier.ac.uk/gus/writing_presenting/academic_posters.html

Extensive list of presentation resources:

- http://sacnas.org/content/presentations-resources

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EXAMPLE

Argonne-Northwestern ANSER Solar Energy Research Center

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Atomic Layer Epitaxy of β-Fe_2O_3 for Photoelectrochemical Water Oxidation

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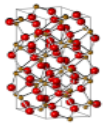
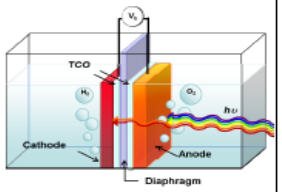
Background

- The conversion of solar energy to chemical energy via photoelectrochemical (PEC) water splitting is a promising route to renewable fuel production.
- Efficient utilization of solar fuels mitigate the negative effects of carbon-based fuel sources.

Hematite (α-Fe_2O_3):
Advantages:
- Suitable band gap
- Earth-abundant
- Stable in aqueous
- Non-toxic

Disadvantages
- Deep $h\nu$ penetration
- Short h^+ diffusion
- High e^-/h^+ recombination
- Slow OER kinetics



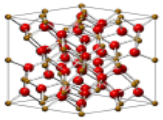


$H_2O \rightarrow \frac{1}{2}O_2 + H_2$ ΔG = 1.23 eV
$2H_2O \rightarrow O_2 + 4H^+ + 4e^-$ (OER)
$2H^+ + 2e^- \rightarrow H_2$ (HER)

Alternate Phase (β-Fe_2O_3):
- Bixbyite crystal structure
- Elusive and metastable
- Unknown PEC properties
- Potential Advantages:
  - Smaller band gap
    - Improved long-λ photoconversion
    - Increased overall efficiency
    - Ideal for tandem absorber cells
  - Differing surface structure
    - Improved OER kinetics
    - Improved catalytic reactivity

Differing bulk properties
- Improved charge transport
- Increase absorption

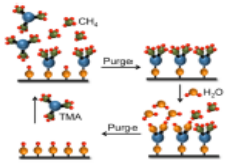
Isomorphic with ITO
- Epitaxy
- Directed crystal growth
- Control of surface truncation
- Improved crystallinity

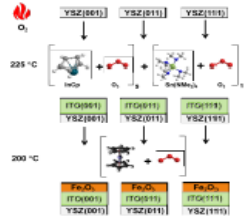


Atomic Layer Deposition

- Self-limiting surface reactions
- Atomic-level control of film thickness and composition
- Phase and structure control
- Conformal coatings on high-aspect ratio nanostructures and large areas
- Low-temperature growth and epitaxy
- Extensive selection of ALD chemistries

Materials	Applications	
Oxides	Electronics	Catalysis
Nitrides	Coating/Protection	Photovoltaics
Metals	Energy Storage	Passivation





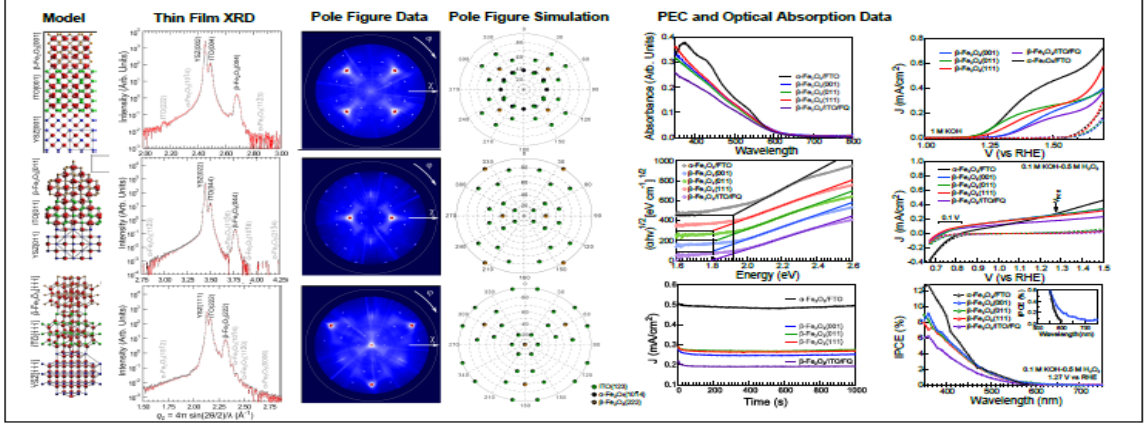
YSZ single crystal substrate
- Annealed at 1100 °C in O_2

ITO
- Common transparent conducting oxide
- Well-studied ALD chemistry
  - $InCp + Sn(NMe_2)_4 + O_2$
- Stable oxide in base (pH > 8)
- ~40nm films
- Resistivity <1×10^{-3} Ω cm

Fe_2O_3
- Well-developed ALD chemistry
  - $FeCp_2 + O_2$
- As-deposited amorphous Fe_2O_3
- PEC-active α-Fe_2O_3 after firing

β-Fe_2O_3 and ITO are isomorphic and lattice-matched (7%)

Results



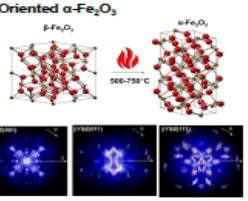
Summary

- Synthesis of pure metastable β-Fe_2O_3 films
- Epitaxial stabilization via isomorphic, transparent, conductive ITO template
- Cube-on-cube-on-cube heterostructure
- Control of crystallite orientation (and termination)

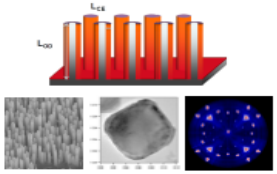
- Epitaxial and polycrystalline films are PEC-active
- β-Fe_2O_3 films show:
  - ~0.1 eV smaller band gap
  - ~0.1 V lower onset potentials
  - Modestly improved >500 nm incident-photon-to-current
  - Stability in 13.6 pH KOH
  - Varying PEC activity associated with surface termination

Future Work

Oriented α-Fe_2O_3



Epitaxial Core-Shell Nanostructures



Acknowledgments

This work was supported as part of the ANSER Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award Number DE-SC0001059. A portion of the research was performed at Argonne National Laboratory, a U.S. Department of Energy, Office of Science, Laboratory operated under Contract No. DE-AC02-06CH11357 by UChicago Argonne, LLC. Use of the Advanced Photon Source (33-BM) was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

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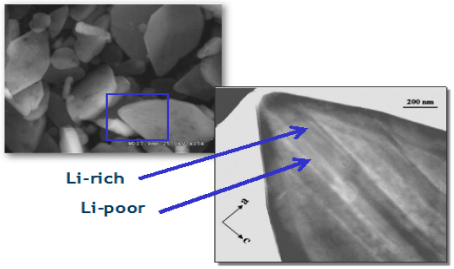
Microstructure of $LiFePO_4$ nanoparticles: The balance of chemistry and stress

M. J. Welland, O. Heinonen, D. Wolf, D. O'Connor, P. Voorhees

Introduction

$FePO_4$ has emerged as a promising cathode material for Li-ion based rechargeable batteries. In particular, nanoparticles have demonstrated high discharge rates and crack resistant microstructures, the mechanisms of which are not completely understood.

Intercalated Li^+ separates into Li-rich and Li-poor phases with different lattice parameters below about 200 °C, which can lead to performance degradation and cracking. This demixing appears to be dependent on the size of the particle, as nanoparticles do not readily demix at lower temperatures.

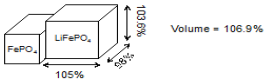


This work seeks to understand the cause and behavior of the striping mechanism to better control charging / discharging and structural behavior. The transition from nanoparticle to bulk behavior will also be explored.

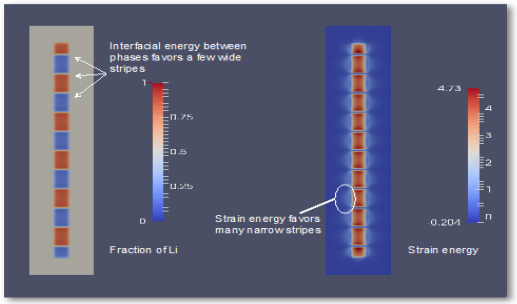
Theory

Li in $FePO_4$ separates into phases of high and low concentration because intermediate concentrations are energetically unfavorable. Interfaces align with crystallographic directions depending on the elastic behavior of the material.

The lattice constants between the two phases is large and anisotropic as shown:

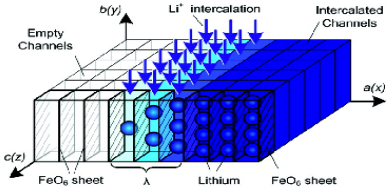


Striping of phases occurs due to a balance between opposing forces of strain and interfacial energy. Interfacial energy drives the system to reduce the number of stripes, and therefore interfaces between phases. Strain energy is minimized by many thin interfaces, which limits the amount of deformation of the inclusion.



Model

Experiments and first principal calculations show diffusion of Li in nanoparticle $FePO_4$ is much faster in the 'b' direction (Pnma), essentially limiting intercalation pathways to channels. This supports 2D simulations perpendicular to these channels. For particles bigger than nano-scale, channels can become blocked and the diffusion reduced, necessitating 3D simulations.



The current work is a Cahn-Hilliard type phase-field model, coupled with linear elasticity. The free energy density and functional are given by:

$$f = \underbrace{cRT\ln c + (1-c)RT\ln(1-c)}_{\text{Ideal mixing}} + \underbrace{\Omega c(1-c)}_{\text{Enthalpy of mixing}} + \underbrace{\frac{1}{2}\sigma : \varepsilon_{el}}_{\text{Strain energy}}$$

$$F = \int_V f + \underbrace{\frac{1}{2}\kappa|\nabla c|^2}_{\text{Gradient energy}}$$

Transport of Li is determined by:

$$\frac{\partial c}{\partial t} = -\nabla \cdot J \qquad J = -\frac{Dc}{RT}\nabla \underbrace{\frac{\delta F}{\delta c}}_{\text{Chem. pot.}}$$

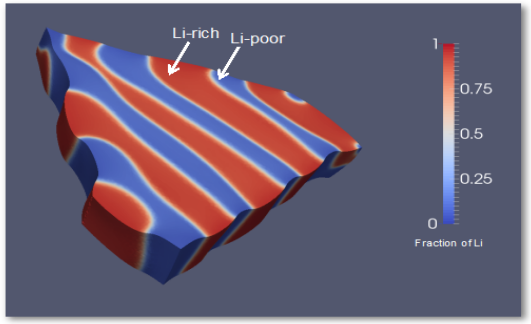
And elastic strain is calculated by:

$$\sigma = C\varepsilon_{el} \qquad \varepsilon_{el} = \varepsilon - c\varepsilon^0$$

The model is implemented in the FEniCS finite element package and run on the Argonne LCRC Blues cluster.

Simulation results

Early results show qualitatively correct stripe formation similar to experimental images. Displacement has been scaled by a factor of 10 for visualization purposes.



This work is supported by:
Argonne National Laboratory LDRD on Mesoscale Elastic Problems
National Physical Sciences Consortium Fellowship

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EXAMPLE

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Salty Water from First Principles

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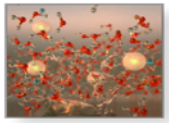
Institute for Molecular Engineering

Abstract

Although water and simple aqueous solutions of salts have been extensively studied both experimentally and theoretically, a complete understanding of their microscopic structure and salt solvation properties is not yet available. One controversial question is the extent to which the presence of ions modifies the water hydrogen-bond network. In addition, the electronic structure of solvated ions has been so far poorly characterized, at least from a first-principles electronic structure perspective. In this work, we performed first-principles simulations of 1 M solutions of Na^+ and Cl^- ions at the gradient-corrected (PBE) and hybrid (PBE0) levels of theory. We examined hydration structure of individual ions and found that Na^+ and Cl^- have different effect on the hydrogen-bond network of water. We also found that the use of hybrid functionals improves the description of the structure and electronic properties of solutions with respect to using semilocal functionals.

Introduction

Knowledge of the structure of water and solutions of salts is important both from fundamental standpoint and for describing many systems and processes of practical significance:



More accurate description of **biologically significant molecules** in solutions of salts (saline)

Systems with interfaces:
- Materials for photocatalytic water splitting;
- Properties of atmospheric aerosols

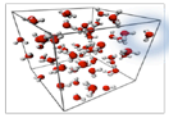
Despite extensive research, many properties of water and solutions of salts are not completely understood, e.g.

Do dissolved salts have long-range effect on the structure of water, or is their effect limited to the first solvation shell of ions?

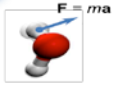
Reason: Experiments cannot probe the structure of hydrogen-bonded liquids directly, they provide only indirect information about the average structure of water and solutions

Simulations, especially from first principles, complement experimental measurements of the structure of water and solutions of salts, and can be used to interpret and validate experiments

First-principles simulations



In molecular dynamics, a few dozens to hundreds molecules are allowed to evolve according to the laws of classical mechanics



First-principles molecular dynamics uses forces computed by density functional theory:

$$\mathbf{F}_i = -\frac{\partial E[\rho]}{\partial \mathbf{R}_i}$$

energy functional (approximated)

Density-functional approximations:

Generalized-gradient approximations (GGA) $E_{XC}^{GGA}[\rho] = E_X^{GGA}[\rho] + E_C^{GGA}[\rho]$ e.g., PBE

exchange correlation

Hybrids $E_{XC}^{hybrid}[\rho] = (1-a)E_X^{GGA}[\rho] + aE_X^{HF} + E_C^{GGA}[\rho]$ e.g., PBE0

Hybrid functionals include a fraction of Hartree–Fock exchange energy, which is very expensive to compute in plane-wave basis sets

Hartree–Fock calculations can be accelerated (2–10x) using recursive subspace bisection

F. Gygi, I. Duchemin, *JCTC* **2013**, 9, 582

Methodology

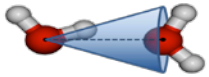
Simulations with PBE functional: 8x20 ps simulations of NaCl, Na^+, Cl^- solutions, as well as pure water; NVT ensemble with Bussi–Donadio–Parrinello (BDP) thermostat at 400 K

Simulations with PBE0: 2x25 ps simulations of NaCl solution; NVT ensemble with BDP thermostat at 380 K

All calculations were done using the Qbox code: **http://eslab.ucdavis.edu/software/qbox/**

Structural properties of Na^+ and Cl^- solutions

Hydrogen bonding in water and solutions of salts

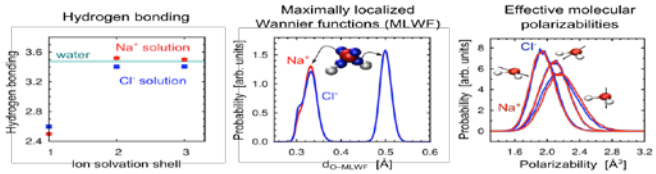


d (O–O) ≤ 3.35 Å; A (H–O–O) ≤ 30°

Total hydrogen bonding from PBE simulations:

Pure water: **3.42±0.04** / H_2O molecule
Aqueous Na^+: **3.42±0.01** / H_2O molecule
Aqueous Cl^-: **3.32±0.03** / H_2O molecule

To understand if the effect of ions is short- or long-ranged, we studied electronic properties of water molecules outside the second solvation shell of ions:



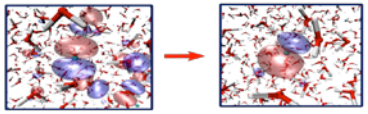
Polarizabilities computed as explained in Q. Wan, L. Spanu, G. Galli, F. Gygi, *JCTC* **2013**, 9, 4124

Cl^- ions have long-range structure-breaking effect on water; Na^+ is neutral/weak structure-maker. We also found that the dipole moment of water is not a sensitive probe of the structure of water

Electronic structure of Cl^- ion in NaCl solutions

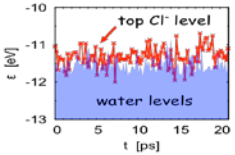
Strategy: Compute orbital energies (ε) for snapshots along a simulated trajectory; identify orbitals belonging to H_2O and Cl^-, and calculate the energy differences (Δε):

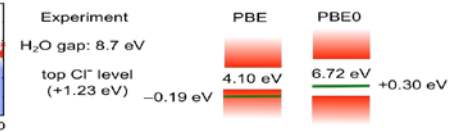
delocalized molecular orbital



localized orbital (MLWF)

We performed this analysis for NaCl solutions using PBE and PBE0 functionals:





Experiment: B. Winter, R. Weber, I. V. Hertel, M. Faubel, P. Jungwirth, E. C. Brown, S. E. Bradforth, *JACS* **2005**, 127, 7203

Best agreement with experiment is when PBE0 is used for **both** simulations and electronic levels. If PBE0 is used only for the levels, H_2O gap changes to 6.59 eV, and Cl^- position—to +0.22 eV

Conclusion: Hybrid functionals are needed to describe electronic properties of solvated anions

Summary and future work

This work is the first ever first-principles illustration that ions can have long-range effect on the structure of water. It supports "traditional" classification of ions as structure makers/breakers

Y. Marcus, *Chem. Rev.* **2009**, 109, 1346

Further experimental and computational studies:
- Planned: X-ray scattering measurements of salty water at the APS with Dr. Chris Benmore
- Simulations of solutions of other salts in water, e.g. LiCl, KBr.

Electronic properties of more realistic systems with air/liquid interface

Acknowledgments:

Argonne NATIONAL LABORATORY — Grant: Incite/VibOSpec

DE-SC0008938

A. P. Gaiduk, C. Zhang, F. Gygi, and G. Galli, *CPL* **604**, 89 (2014)

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Synthesis and Activity of Folate Conjugated Didemnin B for Potential Treatment of Inflammatory Diseases

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[b]Department of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN 47907
[c]Endocyte, Inc., 3000 Kent Ave., West Lafayette, IN, 47906

Abstract

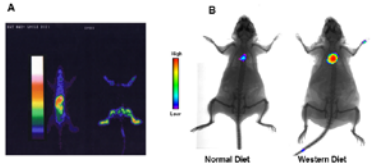
A folate receptor targeted didemnin B conjugate (potent protein synthesis inhibitor) was synthesized using a hydrophilic peptide spacer linked to folate via a releasable disulfide carbonate linker. Cell cytotoxicity and TNF-α inhibition in RAW264.7 macrophage-like cells exhibited IC50s of 13 nM and 5 nM, respectively. Folate didemnin B was found to be ~50-100 fold more potent than didemnin B itself. More importantly, activity of the prodrug was blocked by excess folic acid, demonstrating receptor-mediated cellular uptake of the conjugate.

Background

Receptor Mediated Uptake of Releasable Folate Drugs via the Folate Receptor

(A) Folate receptor (FR) mediated endocytosis of a folic acid drug conjugate. Folate conjugates bind FR with high affinity and are subsequently internalized into endosomes that can reduce disulfide bonds. Within the endosome, a folate-disulfide-drug conjugate is released from the FR and the pro-drug is reduced to liberate the parent drug cargo. Although numerous folate guided DNA synthesis inhibitors and antimitotic agents have been previously synthesized for use against rapidly dividing cancer cells, few agents (e.g. protein synthesis inhibitors such as didemnin B) have been explored for targeting macrophages. (B) Human gamma scintigraphic image demonstrating uptake of folate imaging agents in an arthritic knee (photo courtesy of Endocyte, Inc.).

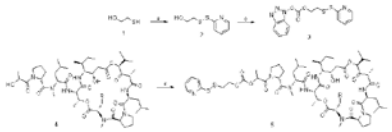
Targeting the Inflammatory Macrophage



(A) EC20-^{99m}Tc uptake in FR+ macrophages localized in arthritic rat limbs (B) Targeting FR+ activated macrophages associated with atherosclerotic plaques in B6.129P2-ApoE^{tm1Unc}/J mice.

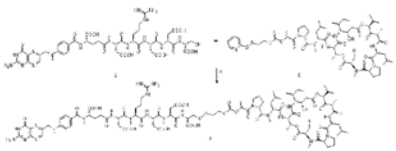
Results

Synthesis of Pyridyldithioethyl Carbonate Didemnin B



Scheme 1. Reagents and conditions: (a) i) MeOC(O)SC(O)CH_2CN, 0 °C, 0.5 h; ii) 2,2'-dipyridyl-disulfide/CH_2CN, 0 °C, 2 h; (b) i) diphosgene, HOBt, TEA/CH_2CN, 0 ° C; ii) s/ 50 ° C, 24 h; (c) 3, DMAP 0 ° C – rt., 2 h. R = p-methoxyphenyl

Synthesis of Completed Drug Conjugate



Scheme 2. Reagents and conditions: (a) (i) H_2O, 0.1 N $NaHCO_3$, pH = 7, r.t. under argon; (ii) 5, pH = 7, r.t. under argon. R = p-methoxyphenyl

Relative Binding Affinity of Folate Peptide Didemnin B

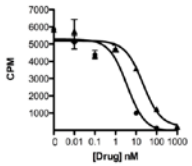


Figure 1. Relative folate receptor binding affinity of folate didemnin B. RAW264.7 cells were incubated for 1 h in the presence of 10 nM ^{3}H-folic acid with increasing competitor concentrations. Black triangles = folate didemnin B. Black circles = folic acid. Relative affinity = 0.14

Dose-response of Folate Didemnin B in RAW264.7 Cells

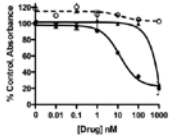


Figure 2. Dose-response of folate didemnin B in RAW264.7 cells. Cells were incubated with increasing concentrations of folate didemnin B in the presence or absence of excess folic acid for 5 h. After another 67 h incubation in fresh media, activity was assessed using the XTT cytotoxicity assay. Meanwhile, Didemnin B activity was measured after 72 h continuous incubation. The results were expressed as % Control in absorbance (mean ± SD in triplicates). Black circles = folate didemnin B (IC50 ~ 13 nM). Open circles = folate didemnin B plus excess folic acid. Black triangles = didemnin B (IC50 ~ 692 nM).

TNF-α Inhibition of Folate Didemnin B in RAW264.7 Cells

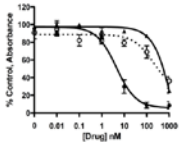


Figure 3. TNF-α inhibition of folate didemnin B in RAW264.7 cells. Cells were incubated with increasing concentrations of folate didemnin B in the presence or absence of excess folic acid for 5 h followed by a 67 h incubation in fresh media. Didemnin B was allowed to incubate for 72 h continuously. E. coli lipopolysaccharide was added 4 h before the end of incubation and TNF-α released in culture media was analyzed by ELISA. The results were expressed as % Control in absorbance (mean ± SD in triplicates). Black circles = folate didemnin B (IC50 ~ 5 nM). Open circles = folate didemnin B plus excess folic acid. Black triangles = didemnin B (IC50 ~ 562 nM).

Conclusions

- A thiol conjugatable form of didemnin B was synthesized.
- Coupling of the didemnin B construct to a folate cysteinyl peptide afforded a releasable, water soluble prodrug.
- The prodrug demonstrated excellent binding affinity, cytotoxicity, and TNF-α inhibition in RAW264.7 cells. TNF-α inhibition appeared to mirror cytotoxicity.
- Future studies will be undertaken to assess whether there is comparable activity in activated peritoneal macrophages.

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EXAMPLE

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