



# Metal-oxo Clusters: Molecular Design from Monomers to Infinity

Hawaii Convention Center 321A

# Dear Colleagues

Happy holidays and welcome to the 6th edition of a polyoxometalate symposium at Pacifichem, spanning 25 years! In 2010, we broadened the Periodic Table confines of this symposium to include uranyl peroxide clusters, which were embraced by both the computational and experimental researchers of the community. Here in 2015, we are inclusive of Group 13 polyoxocation chemistry. Why? Because these often disparate scientific sub-disciplines can learn from each other.

Molecular metal oxo clusters, whether they are group V/VI POMs or from elsewhere on the Periodic Table, all form via strategic control over hydrolysis and condensation reactions. Collectively, we strive to produce molecular metal-oxo clusters from anywhere on the Periodic Table. I am really excited about this symposium because we are seeing progress towards this grand challenge. With synthetic progress comes innovation in function and fundamental understanding, which is also represented here in this symposium. Enjoy, respect, and gain inspiration from the exchange of world-class science that we have the privilege to enjoy in beautiful Hawai'i.

A handwritten signature in black ink, appearing to read "May Ny", with a long horizontal flourish extending to the right.

# Thank you

Please join me in thanking our generous sponsors:

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# Oral Sessions

Hawaii Convention Center 321A

## **Session 7E: POM Building Blocks and Materials**

**THU, Dec 17<sup>th</sup>, 7:00-9:00 pm | Host:** Pedro Molina

## **Session 1P: Fundamental Classic POMs**

**FRI, Dec 18<sup>th</sup>, 1:00-5:00 pm | Host:** Yang-Guang Li

## **Session 5E: Water Oxidation**

**FRI, Dec 18<sup>th</sup>, 7:00-9:00 pm | Host:** Marcella Bonchio

## **Session 2E: Uranium & Polycations**

**SAT, Dec 19<sup>th</sup>, 8:00-12:00pm | Host:** Carles Bo

## **Session 3P: Catalysis, Magnetism & Electrons**

**SAT, Dec 19<sup>th</sup>, 1:00-5:00 pm | Host:** Greta Paztke

## **Session 6E: Noble Metals & Biological Applications**

**SAT, Dec 19<sup>th</sup>, 7:00-9:00 pm | Host:** Debbie Crans

## **Session 4A: Applications & Speciation**

**SUN, Dec 20<sup>th</sup>, 8:00-12:00pm | Host:** John Errington

# Poster Session

Hawaii Convention Center Halls I, II, III

**FRI, Dec 18<sup>th</sup>, 10 am-noon**

**PLEASE ATTEND AND SUPPORT YOUR COLLEAGUES!**

# Symposium Get-togethers

## #79 metal-oxo clusters reception

FRI Dec 17<sup>th</sup> 5:00-7:00 pm, Pa' Kaloka Charlot Courtyard  
(Hawaii Convention Center, [see map](#))

*All symposium attendees and their guests (family members) are welcome.*

## Symposium lunch

SAT Dec 19<sup>th</sup> 12:00-1:00 pm, 321A

*We will be providing a hot buffet lunch. All attendees of the symposium and their guests (family members) are welcome.*

Pacifichem tip #1: eat papaya. It's good for you, local, and in season!



# 7E: POM B. B. & Mat.

THU, Dec 17<sup>th</sup>, 7:00-9:00 pm

## Host: Pedro Molina

**7:00**

Polyoxometalate paneling from  $\{\text{Mo}_2\text{O}_2\text{S}_2\}$  coordination

**Emmanuel Cadot**, *University of Versailles Saint Quentin, France*

**7:20**

Chemistry inside the capsule: Ligand exchange for  $\{\text{W}_{72}\text{Mo}_{60}\}$  keplerate

**Vladimir Korenev**, *Nikolaev Institute of Inorganic Chemistry, Russia*

**7:40**

Electrical conduction of polyoxometalate-based solid:  
Non-covalent wiring of clusters to networks

**Ryo Tsunashima**, *Yamaguchi University, Japan*

**8:00**

Polyoxometalate complexes of anatase- $\text{TiO}_2$  cores in water.

**Ira Weinstock**, *Ben Gurion University, Israel*

**8:20**

Visible-light-responsive photoredox catalysis of silicotungstates

**Kosuke Suzuki**, *University of Tokyo (School of Engineering), Japan*

**8:40**

Construction of polyoxometalate-based porous materials  
for heterogeneous catalysis

**Yang-Guang Li**, *Northeast Normal University, USA*

# 1P: Fund. Classic POMs

FRI, Dec 18<sup>th</sup>, 1:00-5:00 pm

## Host: Yang-Guang Li

**1:00**

Computational approach to giant POMs and new POCATs

**Carles Bo**, *Institute of Chemical Research of Catalonia (ICIQ), Spain*

**1:25**

Hydrogen-bonded trimer of methylated molybdoplatinate

**Atsushi Yagasaki**, *Kwansei Gakuin University, Japan*

**1:45**

Zr-cluster substituted poly(polyoxometalate)s made by synergistic structure-directing roles

**Guo-Yu Yang**, *Beijing Institute of Technology, China*

**2:05 (Flash-poster presentation)**

Driving polyoxometalates to dense thin films: TMA<sup>+</sup> vs. H<sup>+</sup>

**Ryan Mansergh**, *Oregon State University (CSMC), USA*

**2:10 (Flash-poster presentation)**

Novel phosphonium and ammonium hexatungstate compounds for the precursor of inorganic photoresists

**Sumit Saha**, *Oregon State University (CSMC), USA*

**2:15**

All-inorganic metallacrowns by heteropolyoxovanadates

**Yoshihito Hayashi**, *Kanazawa University, Japan*

**2:35**

Turning up the heat on reductive polyoxometalate synthesis: benefits of COST action CM1203 (PoCheMoN)

**John Errington**, *Newcastle University, UK*

# 1P: Fund. Classic POMs

FRI, Dec 18<sup>th</sup>, 1:00-5:00 pm

## Host: Yang-Guang Li

**2:55**

Interconversion among neutral vanadium(V) oxo cluster complexes by changing the solvent systems

**Shintaro Kodama**, *Chuo University, Japan*

**3:15**

Bridging the opposite chemistries of tantalum and tungsten polyoxometalates

**Pedro Molina**, *Oregon State University, USA*

**3:35**

Synthesis and application of molybdenum oxides containing polyoxomolybdate building units

**Masahiro Sadakane**, *Hiroshima University, Japan*

**3:55**

Chemistry of solution to film: amorphous niobium phosphate thin films from acidic aqueous precursors

**Deok-Hie Park**, *Oregon State University (CSMC), USA*

**4:15**

Inorganic-organic hybrid assembled materials based on block copolymers and polyoxometalates

**Jie Zhang**, *Peking University, China*

**4:35**

Polyoxometalate mediated oxidative transformations

**Ronny Neumann**, *Weizmann Institute of Science, Israel*



# 5E: Water Oxidation

FRI, Dec 18<sup>th</sup>, 7:00-9:00 pm

## Host: Marcella Bonchio

**7:00**

Computational study of the water oxidation mechanism catalyzed by the polyanion  $[\text{Co}_4(\text{H}_2\text{O})_2(\text{XW}_9\text{O}_{34})_3]^{10-}$  ( $\text{X} = \text{P}^{5+}, \text{V}^{5+}$ )

**Joaquín Soriano-López**, *Institute of Chemical Research of Catalonia (ICIQ), Spain*

**7:20**

Natural born catalysts: The great POM beauty

**Marcella Bonchio**, *University of Padova, Italy*

**7:40**

Water-oxidation catalysis starting with cobalt polyoxometalates: Addressing the challenging, "who's the true catalyst?" question

**Richard Finke**, *Colorado State University, USA*

**8:00**

Polyoxometalate catalyst design for water oxidation and reduction

**Greta Patzke**, *University of Zurich, Switzerland*

**8:20**

Catalytic water oxidation with cobalt-containing POMs: processing and activity in the solid state and into plastic thin films

**José Ramón Galán-Mascarós**, *Institute of Chemical Research of Catalonia (ICIQ), Spain*

**8:40**

Polyoxometalate catalysts for solar fuel production

**Craig Hill**, *Emory University, USA*

# 2E: Uranium & Polycations

SAT, Dec 19<sup>th</sup>, 8:00am-12:00pm

## Host: Carles Bo

**8:00**

Oxygen-isotope exchanges in nanometer-sized ions as a window into geochemical processes

**William Casey**, *University of California (Davis), USA*

**8:25**

Chemistry of tetravalent actinide (U and Th) carboxylates: isolation of oxo/hydroxo polynuclear clusters

**Clément Falaise**, *Oregon State University, USA*

**8:45**

Lanthanide "Bottlebrush" clusters

**Massimiliano Massi**, *Curtin University, Australia*

**9:05**

Designer polyoxometalate — silver alkynide chimera cluster

**Tomoji Ozeki**, *Nihon University, Japan*

**9:25**

Withdrawn

**9:35**

Structures and properties of uranyl peroxide cage clusters

**Peter Burns**, *University of Notre Dame, USA*

**10:00**

Structural variations in Group 13 heteropolycations

**Tori Forbes**, *University of Iowa, USA*

# 2E: Uranium & Polycations

SAT, Dec 19<sup>th</sup>, 8:00am-12:00pm

## Host: Carles Bo

**10:20**

Group 13 (<sup>27</sup>Al, <sup>71</sup>Ga) studies of metal-oxide clusters

**Blake Hammann**, *Washington University (St Louis), USA*

**10:35**

Novel hybrid uranium-transition metal peroxide nanoclusters

**Jie Qiu**, *University of Notre Dame, USA*

**10:50**

Metal(IV)-oxide cluster formation: Understanding and controlling hydrolysis

**Lynn Soderholm**, *Argonne National Laboratory, USA*

**11:15**

Solid-state dynamics and hydrogen bonding in uranyl clusters using multi-nuclear MAS NMR spectroscopy

**Todd Alam**, *Sandia National Laboratories, USA*

**11:35**

Main group coordination clusters: Synthesis, solution speciation, structure and their use as "inks" for oxide materials

**Darren Johnson**, *University of Oregon, USA*

# 3P: Cat., Magn. & Electrons

SAT, Dec 19<sup>th</sup>, 1:00-5:00 pm

## Host: Greta Paztke

**1:20**

Molecular cluster batteries of nano-hybrid materials between POMs and nanocarbons

**Kunio Agawa**, *Nagoya University, Japan*

**1:45**

Electron transfer properties through monolayers of polyoxometalates covalently immobilized on electrodes

**Anna Proust**, *Pierre and Marie Curie University, France*

**2:15**

Magnetic POMs in molecular spintronics and quantum computing

**Eugenio Coronado**, *University of Valencia, Spain*

**2:45**

Withdrawn

**2:55**

Localized and delocalized excited states in Ti<sub>6</sub> and Ti<sub>17</sub> polyoxotitanate clusters

**Piotr Piotrowiak**, *Rutgers University, USA*

**3:15**

Photoreduction process of nucleotide-coordinated polyoxomolybdates (Flavin)

**Eri Ishikawa**, *Chubu University (College of Engineering), Japan*

# 3P: Cat., Magn. & Electrons

SAT, Dec 19<sup>th</sup>, 1:00-5:00 pm

## Host: Greta Paztke

**3:35**

Break / Discussion

**3:40**

Using Fourier-transformed AC voltammetry to provide new insight into electrocatalysis with polyoxometalates

**Alan Bond**, *Monash University, Australia*

**4:05**

Redox-induced selective uptake-release of cations in porous ionic crystal based on polyoxomolybdates

**Sayaka Uchida**, *University of Tokyo, Japan*

**4:25**

The iron Keggin from water

**May Nyman**, *Oregon State University, USA*

**4:45**

Cation-induced conformational changes in uranyl-peroxide nanoclusters and their effect on anion molecular dynamics

**Mateusz Dembowski**, *University of Notre Dame, USA*

# 6E: Noble Met. & Bio. Appl.

SAT, Dec 19<sup>th</sup>, 7:00-9:00 pm

## Host: Debbie Crans

**7:00**

Self-assembly of polyoxometalates for flexible ionic organic frameworks

**Lixin Wu**, *Jilin University, China*

**7:20**

Distortions in decavanadates and how that may impact interactions with biological interfaces

**Debbie Crans**, *Colorado State University, USA*

**7:40**

Polyoxometalates as a novel class of artificial proteases

**Tatjana Parac-Vogt**, *KU Leuven, Belgium*

**8:10**

Recent developments in polyoxo-noble-metalate chemistry

**Ulrich Kortz**, *Jacobs University, Germany*

**8:30**

Understanding the assembly of gigantic polyoxometalate clusters with information theory and symmetry

**Lee Cronin**, *University of Glasgow, UK*

# 4A: Appl. & Speciation

SUN, Dec 20<sup>th</sup>, 8:00-12:00 pm

## Host: John Errington

**8:00**

Polyoxometalate complexes with coordinated main group elements (Pb and Bi)

**Sergey Adonin**, *Nikolaev Institute of Inorganic Chemistry, Russia*

**8:20**

Chemical and electrochemical condensation of polyoxometalates with nanocrystals for solution processed electrochromic "smart windows"

**Delia Milliron**, *University of Texas (Austin), USA*

**8:40**

Vanadium-based polyoxometalate as cathode-active materials for Li-ion batteries

**Pablo Aparicio**, *Rovira i Virgili University, Spain*

**9:00**

Oxohydroxometal clusters: speciation, film properties, and nanopatterning

**Doug Keszler**, *Oregon State University (CSMC), USA*

**9:25**

Withdrawn

**9:45**

Probing ion-pairing trends of polyoxometalates with counter-cation <sup>133</sup>Cs NMR

**Dylan Sures**, *Oregon State University, USA*

# 4A: Appl. & Speciation

SUN, Dec 20<sup>th</sup>, 8:00-12:00 pm

## Host: John Errington

**10:05**

Selective uptake of Cs<sup>+</sup> by porous ionic crystals based on redox of polyoxometalates

**Saori Seino**, *University of Tokyo, USA*

**10:25**

A high-nuclear vanadoniobate {Nb<sub>48</sub>V<sub>8</sub>} double-decker wheel

**Xin-Long Wang**, *Institute of Functional Material Chemistry, China*

**10:45**

Hafnium-oxo clusters: the atomic structure behind high-resolution patterning

**Sara Goberna-Ferrón**, *Oregon State University (CSMC), USA*

**11:05**

Polyoxotungstates in photocatalysis

**Josep M. Poblet**, *Rovira i Virgili University, Spain*

**11:35**

Macroion-Macroion attraction - the roles of counterions, co-ions and water structures

**Tianbo Liu**, *University of Akron, USA*



# Poster Session

FRI, Dec 18<sup>th</sup>, 10:00-12:00 pm

## Location: Halls I, II, and III

The pH dependence of molecular structures of Dawson-type tri-aluminum-substituted polyoxotungstates

**Motoko Aikawa**, *Shizuoka University, Japan*

Hydration of Diphenylacetylene Catalyzed by Phosphanegold(I) Cationic Species Stabilized with Polyoxoanion

**Hidekazu Arai**, *Kanagawa University, Japan*

Mode of action of decavanadate in biology

**Debbie Crans**, *Colorado State University, USA*

Elucidation of the fast self-assembly of the uranyl peroxide cluster  $\{U_{32}\}$

**Clément Falaise**, *Oregon State University, USA*

Lindqvist polyoxoniobates as aqueous precursors for lithium niobate thin films

**Dylan Fast**, *Oregon State University (CSMC), USA*

Polyoxometalates to metal oxide thin film: the effect of protonation

**Lauren Fullmer**, *Oregon State University (CSMC), USA*

Keggin-type platinum(II)-coordinated polyoxotungstates: Syntheses, molecular structures, and photocatalytic performance for hydrogen evolution from water under visible light irradiation

**Yuki Ihara**, *Shizuoka University, Japan*

# Poster Session

FRI, Dec 18<sup>th</sup>, 10:00-12:00 pm

## Location: Halls I, II, and III

Molecular chirality and racemization behavior of sandwich-type polyoxometallolanthanoates

**Jun Ijima**, *Nihon University, Japan*

Reversible structural conversion of chloride-incorporated dodecavanadates for release control of the chloride

**Yoshitaka Inoue**, *Kanazawa University, Japan*

Open-Dawson polyoxometalates containing tetraaluminum, tetragallium and decaindium hydroxide clusters

**Yusuke Inoue**, *Kanagawa University, Japan*

Visible-light-responsive multielectron redox catalysis utilizing electron transfer from coordinated alcohols to lacunary polyoxometalates

**Jinu Jeong**, *University of Tokyo (School of Engineering), Japan*

Evaluation of a structural ion fluctuation in Preyssler-type polyoxometalate salt

**Chisato Kato**, *Hiroshima University, Japan*

Syntheses, molecular structures, and acid catalysis of organozirconium complexes with Keggin-type mono-aluminum mono-aluminum-substituted polyoxotungstates

**Sakie Kato**, *Shizuoka University, Japan*

# Poster Session

FRI, Dec 18<sup>th</sup>, 10:00-12:00 pm

## Location: Halls I, II, and III

Mesoporous ionic crystals constructed with cationic metal complexes ( $\text{Cr}^{3+}$ ,  $\text{Fe}^{3+}$ ) and anionic polyoxometalates: Importance of water clusters as templates

**Ryosuke Kawahara**, *University of Tokyo, Japan*

Control of composition and structure in decavanadate-alkylamine hybrid layered crystals

**Yoshiki Kiyota**, *Tokai University (School of Science), Japan*

Syntheses of inorganic-organic hybrid crystals composed of octamolybdates and heterocyclic surfactants

**Jun Kobayashi**, *Tokai University (School of Science), Japan*

Cobalt-polyoxometalates as oxidation co-catalysts in photocatalytic  $\text{H}_2$  evolution

**Fengyan Li**, *Northeast Normal University, China*

A new organic-inorganic hybrid based on dimeric  $[\text{Mn}_2\text{V}_{22}\text{O}_{64}]^{10-}$  polyoxoanion

**Ying Lu**, *Northeast Normal University, China*

Driving polyoxometalates to dense thin films:  $\text{TMA}^+$  vs.  $\text{H}^+$

**Ryan Mansergh**, *Oregon State University (CSMC), USA*

Construction of manganese and cobalt cores stabilized in polyoxovanadate ligands

**Tatsuya Maruyama**, *Kanazawa University, Japan*

# Poster Session

FRI, Dec 18<sup>th</sup>, 10:00-12:00 pm

## Location: Halls I, II, and III

Open-Dawson polyoxometalate containing mixed-valence trimanganese cluster

**Satoshi Matsunaga**, *Kanagawa University, Japan*

Inorganic anionic cage  $[\alpha\text{-Si}_2\text{W}_{18}\text{O}_{62}]^{8-}$  with reversible proton capturing inside the aperture via intramolecular hydrogen bonds

**Takuo Minato**, *University of Tokyo, Japan*

Synthesis of heterogeneous catalyst composed of aluminum hydroxide cluster polycation and  $[\text{SiV}_3\text{W}_9\text{O}_4]^{7-}$

**Kosuke Mizuno**, *University of Tokyo, Japan*

Synthesis of heterogeneous catalysts composed of aluminum hydroxide cluster and  $[\text{CoW}_{12}\text{O}_4\text{O}]^{6-}$

**Takuto Mura**, *University of Tokyo, Japan*

$[\text{MO}_4]^{2-}$  (M = Mo, W) encapsulating silver(I) ethynide clusters formed by template exchange reactions abstracting  $[\text{MO}_4]^{2-}$  groups from the Keggin-type polyoxometalates

**Kenji Ohashi**, *Nihon University (College of Humanities and Sciences), Japan*

Novel phosphonium and ammonium hexatungstate compounds for the precursor of inorganic photoresists

**Sumit Saha**, *Oregon State University (CSMC), USA*

# Poster Session

FRI, Dec 18<sup>th</sup>, 10:00-12:00 pm

## Location: Halls I, II, and III

Construction of chiral polyoxometalate/nanoparticle composites toward chirality transfer and enhancement

**Lei Shi**, *Jilin University, China*

Modification of zirconium-substituted polyoxometalates for peroxidase-like catalysis

**Yong-Hui Wang**, *Northeast Normal University, China*

Liquid-crystalline materials with an inorganic core in mesogen

**Ryohei Watanabe**, *Ritsumeikan University, Japan*

Thermodynamic stability of aqueous metal clusters: a dynamic approach

**Lindsay Wills**, *Oregon State University, USA*

Base catalysis of niobate clusters

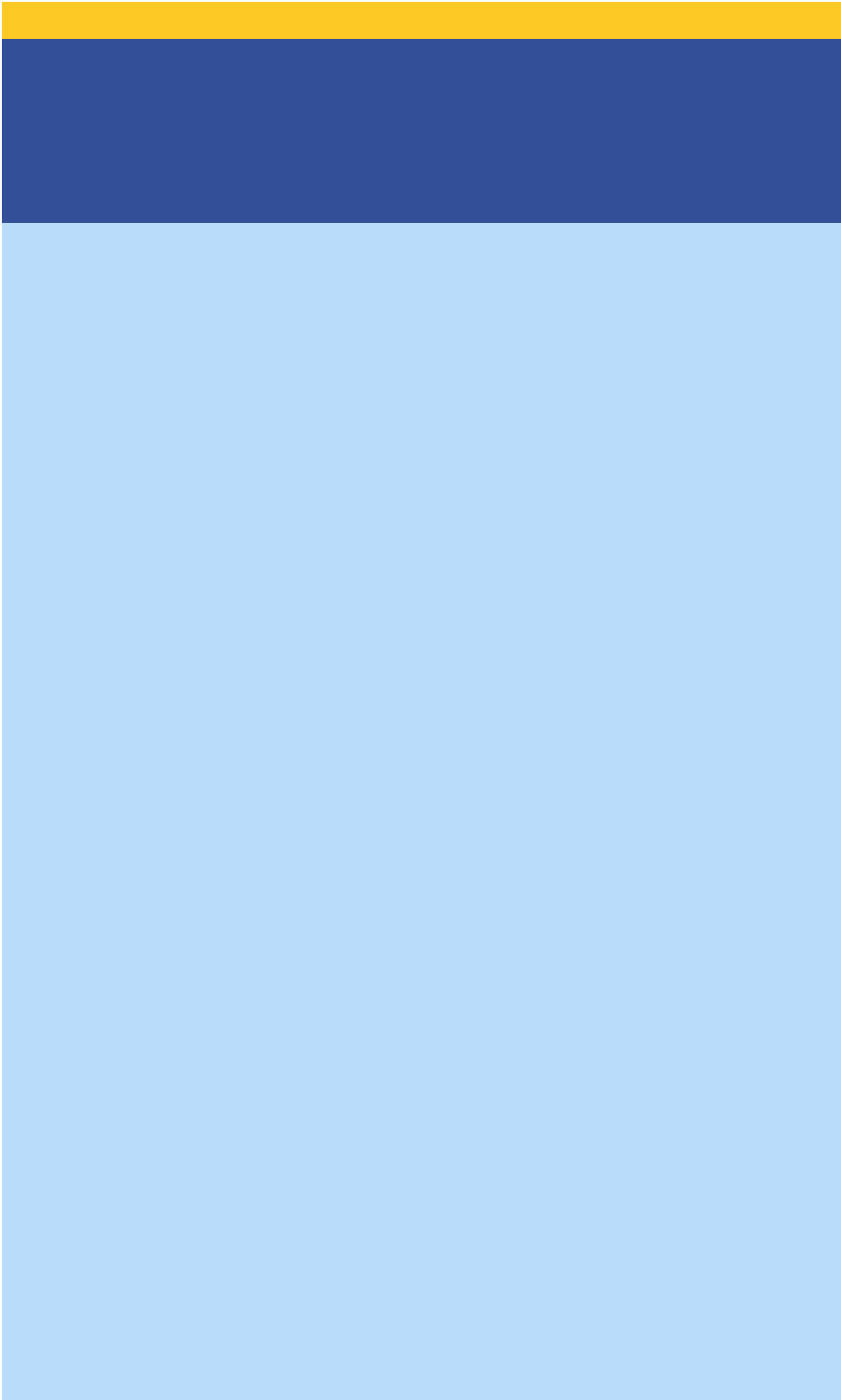
**Seiji Yamazoe**, *University of Tokyo, Japan*

Assembly of coordination-adjustable units to form inorganic-organic hybridized molecular-scale proton conductors

**Hongying Zhang**, *Northeast Normal University, China*

Synthesis and characterization of Sb-bicapped heteropolyoxoniobate microtube

**Zhe-Yu Zhang, Jun Peng & Wan-Li Zhou**, *Northeast Normal University, China*





**Pacifichem tip #2: when you've had enough of science, go to Hanauma Bay and meet a Humuhumunukunuuapua!**

**HAPPY HOLIDAYS AND SAFE TRAVELS BACK HOME!!**

*This brochure was designed and assembled by Pedro Molina (@scifanz), Amanda Polley, Sharon Betterton and May Nyman. We hope you liked it and found it useful. Mahalo!*

