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14. ABSTRACT Kevin Leung, Ph.D. from Sandia National Lab and Oleg Borodin, Ph.D. from the Army Research Laboratory organized the "Modeling and Simulations of Electrochemical Interfaces and Materials for Energy Storage" symposium within the Computers in Chemistry (COMP) Division of the American Chemical Society at the 248th National Meeting in San Francisco (August 11-14, 2014). The invited speakers of the symposium are considered key researchers in their fields and provided an equal mix of computational and experimental research. This resulted in an excellent symposium that allowed the audience and speakers to see the merging of the computational and					
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Report Title

Final Report: A request for the CONFERENCE AND SYMPOSIA GRANT from COMP division of American Chemical Society

ABSTRACT

Kevin Leung, Ph.D. from Sandia National Lab and Oleg Borodin, Ph.D. from the Army Research Laboratory organized the "Modeling and Simulations of Electrochemical Interfaces and Materials for Energy Storage" symposium within the Computers in Chemistry (COMP) Division of the American Chemical Society at the 248th National Meeting in San Francisco (August 11-14, 2014). The invited speakers of the symposium are considered key researchers in their fields and provided an equal mix of computational and experimental research. This resulted in an excellent symposium that allowed the audience and speakers to see the merging of the computational and experimental research worlds that thus push each other's research.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

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Paper

TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received

Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 40.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

<u>NAME</u>	<u>PERCENT_SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT_SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

Names of Under Graduate students supported

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in
science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue
to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for
Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work
for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive
scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

Technology Transfer



248th ACS National Meeting and Exposition
August 10-14, 2014, San Francisco, CA
Chemistry and Global Stewardship

Divisions

Return to: [Divisions](#) -> [Sessions](#)

COMP

Emilio Esposito, Scott Wildman

Monday, August 11, 2014

Oral Session

Modeling and Simulations of Electrochemical Interfaces and Materials for Energy Storage - AM Session

Aqueous and Other Interfaces, Energy Conversions, and Electrochemical Reactions

Location: Moscone Center, West Bldg.

Room: 2009

Cosponsored by: PHYS

Organizers: Kevin Leung, Oleg Borodin

Presiders: Dat Tran, Stephen Harris

Duration: 8:30 am - 12:05 pm

Pres Time	Pub #	Presentation Title
8:30 am	88	First-principles modeling of electrochemical interfaces for energy storage Axel Gross , Nicolas Hoermann, Markus Jaeckle, Florian Gossenberger, Katrin Forster-Tonigold, Sung Sakong, Tanglaw Roman.
9:05 am	89	Structure, pKa, and vibrational signatures of oxide/water interfaces, including electrolytes, from first principles DFT-MD simulations Marie-Pierre Gaigeot , Marialore Sulpizi, Michiel Sprik.
9:40 am	90	Microscopic characterization of the fluorite/water interface from theory and experiments Rémi Khatib, Maria J Perez-Haro, Ellen HG Backus, Marie-Pierre Gaigeot, Marialore Sulpizi .
10:15 am		Intermission
10:30 am	91	Li ion transport, via time-resolved spatial Li maps, in Li-ion battery electrodes Stephen J. Harris
11:05 am	92	Insights into the influence of water ions at an aqueous electrode interface John A Kattirtzi , Adam P Willard.
11:25 am	93	Light absorbers for photoelectrochemical energy conversion: First principles calculations Giulia Galli
12:00 pm		Concluding Remarks

COMP

Emilio Esposito, Scott Wildman

Monday, August 11, 2014

Oral Session

Modeling and Simulations of Electrochemical Interfaces and Materials for Energy Storage - PM Session

Fundamentals of Electrochemical Reactions at Interfaces

Location: Moscone Center, West Bldg.

Room: 2009

Cosponsored by: PHYS

Organizers: Kevin Leung, Oleg Borodin

Presiders: Marialore Sulpizi, Michael Sprik

Duration: 1:30 pm - 5:25 pm

Pres Time	Pub #	Presentation Title
1:30 pm		Introductory Remarks

1:35 pm	125	WITHDRAWN
2:10 pm	126	First-principles molecular dynamics simulations on electrochemical reactions using effective screening medium method Minoru Otani
2:45 pm	127	Towards simulations of electrochemical interfaces in graphene-based supercapacitors under realistic operating conditions Brandon C. Wood
3:20 pm		Intermission
3:35 pm	128	Theoretical modeling of electrode/electrolyte interface from first-principles periodic continuum solvation (DFT/CM-MPB) method Zhi-Pan Liu
4:10 pm	129	Activation of the OH bond of water and hydroxide groups adsorbed at transition metal oxide interfaces Michiel Sprik , John Kattirtzi, Joost VandeVondele, Jun Cheng.
4:45 pm	130	Oxidation stability and decomposition reactions of battery electrolytes and additives in bulk and at interfaces Oleg Borodin , Marco Olguin, T. Richard Jow, Carrie Spear, Jaroslaw Knap, Kenneth Leiter.
5:05 pm	131	Ab initio molecular dynamics simulations of electrolyte electrochemical reactions on battery electrode surface Kevin Leung
5:20 pm		Concluding Remarks

COMP**Emilio Esposito, Scott Wildman****Tuesday, August 12, 2014****Oral Session**

Modeling and Simulations of Electrochemical Interfaces and Materials for Energy Storage - AM Session

Battery Materials and Interfaces (Mostly Electrodes)

Location: Moscone Center, West Bldg.

Room: 2009

Cosponsored by: PHYS

Organizers: Kevin Leung, Oleg Borodin

Presiders: Axel Gross, Donald Truhlar

Duration: 8:30 am - 12:20 pm

Pres Time	Pub #	Presentation Title
8:30 am	165	Combining first principles computation and X-ray, neutron, and electron scattering for understanding and designing next generation battery materials Shirley Meng
9:05 am	166	Nanostructured composite electrodes for Li-ion batteries with enhanced energy density Naoki Nitta, Feixiang Wu, Kara Evanoff, Jung Tae Lee, Daniel Gordon, Wentian Gu, Jim Benson, Alexandre Magasinski, Igor Kovalenko, Hyea Kim, Gleb Yushin .
9:40 am	167	First principles design of lithium superionic conductors Shyue Ping Ong , Yifei Mo, William D Richards, Lincoln Miara, HyoSug Lee, Gerbrand Ceder.
10:15 am		Intermission
10:30 am	168	Elucidating electrode and solid electrolyte kinetics from first principles Anton Van der Ven
11:05 am	169	Quantum chemistry of lithium-ion battery cathodes Bo Wang, Donald G. Truhlar .
11:40 am	170	WITHDRAWN
12:15 pm		Concluding Remarks

COMP**Emilio Esposito, Scott Wildman****Tuesday, August 12, 2014**

Oral Session

Modeling and Simulations of Electrochemical Interfaces and Materials for Energy Storage - PM Session

Battery Materials and Interfaces (Interfaces, SEI, Electrolytes)

Location: Moscone Center, West Bldg.

Room: 2009

Cosponsored by: PHYS

Organizers: Kevin Leung, Oleg Borodin

Presiders: Oleg Borodin

Duration: 1:30 pm - 5:25 pm

Pres Time	Pub #	Presentation Title
1:30 pm	204	Interfacial phenomena and chemical cross-talk in $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$/graphite Li-ion battery system Robert Kostecki, A. Jarry, Y. Fu, M. Ayache, Vincent S. Battaglia.
2:05 pm	205	Additive effect on initial stage of solid electrolyte interphase (SEI) formation in lithium ion battery Yoshitaka Tateyama, Keisuke Ushirogata, Keitaro Sodeyama, Yukihiro Okuno.
2:40 pm	206	Insight into structure and transport of carbonate, nitrile electrolytes, and SEI components Oleg Borodin, Marco Olguin, Joshua Allen, Wesley Henderson.
3:00 pm		Intermission
3:15 pm	207	Modeling solid-electrolyte interfacial reactions on Si anodes of Li-ion batteries Perla B Balbuena, Julibeth M Martinez de la Hoz, Yuguang Ma.
3:50 pm	208	Defect facilitated electron leakage through the solid electrolyte interphase in Li-ion batteries Yue Qi
4:25 pm	209	Molecular dynamics simulations of carbonates based electrolytes at charged surfaces Dmitry Bedrov, Jenel Vatamanu, Mihaela Vatamanu, Oleg Borodin.
5:00 pm	210	Molecular vesicles as battery electrodes Hal Gokturk
5:20 pm		Concluding Remarks

COMP**Emilio Esposito, Scott Wildman****Wednesday, August 13, 2014****Oral Session**

Modeling and Simulations of Electrochemical Interfaces and Materials for Energy Storage - AM Session

Electrolyte Stability in Li-ion and Beyond Li Batteries

Location: Moscone Center, West Bldg.

Room: 2009

Cosponsored by: PHYS

Organizers: Kevin Leung, Oleg Borodin

Presiders: William Swope

Duration: 8:30 am - 11:55 am

Pres Time	Pub #	Presentation Title
8:30 am	415	Theoretical analysis of fundamental limitations of lithium-air batteries Venkat Viswanathan
9:05 am	416	Computational study of the electrochemical stability of solvents for Li/air batteries Hans W Horn, Julia E Rice, William C Swope, Jeannette M Garcia, Ho-Cheol Kim, Winfried W Wilcke, Robert D Miller, Alan C Luntz, Takashi Mori, Gregory M Wallraff.
9:40 am	417	WITHDRAWN
10:00 am		Intermission
10:15 am	418	Electronic structure of interfaces and their role in charge and discharge chemistries in lithium-oxygen batteries Larry A Curtiss, Kah Chun Lau, Rajeev Assary, Lei Cheng, Ujjal Das, Paul Redfern.
10:50 am	419	Structure optimization and new design of nanoparticles for electrocatalytic oxygen reduction Wei Guangfeng, Zhi-Pan Liu.

11:10 am	420	DME decomposition on Li₂O₂ surfaces: Role of peroxide and superoxide terminations Nitin Kumar , Maxwell D. Radin, Donald J. Siegel.
11:30 am	421	Computational studies on electrolyte degradation in aprotic Li-air battery by in situ generated oxidative (oxygen or oxidizing) species Vincent K C Chau , Kwong Yu Chan, Hao Hu.
11:50 am		Concluding Remarks

COMP**Emilio Esposito, Scott Wildman****Wednesday, August 13, 2014****Oral Session**

Modeling and Simulations of Electrochemical Interfaces and Materials for Energy Storage - PM Session

Multiscale and Multiphysics Modeling

Location: Moscone Center, West Bldg.

Room: 2009

Cosponsored by: PHYS

Organizers: Kevin Leung, Oleg Borodin

Presiders: De-en Jiang, Sreekanth Pannala

Duration: 1:30 pm - 5:30 pm

Pres Time	Pub #	Presentation Title
1:30 pm	455	WITHDRAWN
2:05 pm	456	Subspace-corrected functionals for linear-scaling density functional theory simulation of extended energy storage interfaces Gilberto Teobaldi , Benjamin J Morgan, David D O`Regan, Nicholas D Hine, Arash A Mostofi.
2:40 pm	457	WITHDRAWN
3:00 pm		Intermission
3:15 pm	458	Multiscale modeling approach for performance and safety of lithium-ion batteries Sreekanth Pannala , John A Turner, Srikanth Allu, Wael R. Elwasif, Sergiy Kalnaus, Srdjan Simunovic, Jay J. Billings, Hsin Wang, Jagjit Nanda.
3:50 pm	459	Multi-scale simulation of electrode interfaces Thomas F Miller
4:25 pm	460	Toward efficient electrochemical conversion of CO₂: Catalyst design accelerated by simulation-based screening Hyungjun Kim , Hyung-Kyu Lim, Hyeyoung Shin, William A Goddard III.
4:45 pm	461	Modifying MOFs for specific adsorption interactions: The cases of H₂ and CH₄ Ehud Tsivion , Jarad A. Mason, Bess Vlasisavljevich, Zeric Hulvey, Craig M. Brown, Berend Smit, Jeffrey R. Long, Martin Head-Gordon.
5:05 pm	462	Nature of electro-osmosis in hydrated polymer electrolyte membranes Yoong-Kee Choe
5:25 pm		Concluding Remarks

COMP**Emilio Esposito, Scott Wildman****Thursday, August 14, 2014****Oral Session**

Modeling and Simulations of Electrochemical Interfaces and Materials for Energy Storage - AM Session

Non-Faradic Energy Storage, Interfacial Structure

Location: Moscone Center, West Bldg.

Room: 2009

Cosponsored by: PHYS

Organizers: Oleg Borodin, Kevin Leung

Presiders: Oleg Borodin

Duration: 8:30 am - 12:05 pm

Pres Time	Pub #	Presentation Title
8:30 am	493	WITHDRAWN
9:05 am	494	Understanding supercapacitors De-en Jiang
9:40 am	495	How to improve the non-Faradic energy densities in C-based conductive nanopores? Insights from atomistic simulations Jenel Vatamanu , Dmitry Bedrov.
10:15 am		Intermission
10:30 am	496	WITHDRAWN
11:05 am	497	Computational analysis and prediction of the interfacial structure and capacitance of nanostructured carbon electrodes in an ionic liquid electrolyte Gyeong S Hwang , Alexander J Pak, Eunsu Paek.
11:40 am	498	Molecular dynamics studies on the Electrical Double layer at the liquid/electrode interface Jose L Mendoza-Cortes , Nahid P Khiabani, William A Goddard III.
12:00 pm		Concluding Remarks
