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# RPPR Final Report

## as of 19-May-2020

Agency Code:

Proposal Number: 73255CHCF

**Agreement Number: W911NF-18-1-0171**

### INVESTIGATOR(S):

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**Email:** dts@uw.edu  
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**Principal:** Y

Organization: **The Electrochemical Society**

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Country: USA

DUNS Number: 067386755

EIN: 131771269

**Report Date:** 09-Aug-2019

Date Received: 19-May-2020

**Final Report** for Period Beginning 10-May-2018 and Ending 09-May-2019

**Title:** ECS Data Sciences Hack Week--Seattle 2018

**Begin Performance Period:** 10-May-2018

**End Performance Period:** 09-May-2019

**Report Term:** 0-Other

Submitted By: Ngoc Le

Email: development@electrochem.org

Phone: (609) 737-1902

**Distribution Statement:** 1-Approved for public release; distribution is unlimited.

### STEM Degrees:

### STEM Participants:

**Major Goals:** ARO funding was used to partially support 28 participants, mostly early career scholars, at ECS Data Science Hack events at the 233rd and 10 participants at the AiMES meetings of the electrochemical society.

**Accomplishments:** Hack Week

<https://www.electrochem.org/233/hack-week>

Building on the success of the first ECS Data Sciences Hack Day (October 2017), ECS is offered another opportunity at the ECS spring meeting in Seattle. In May 2018, the program expanded to an entire week as the next stage in ECS supporting a growing electrochemical data science and open source community. The goal of the event was to increase awareness and impact of data science tools, open source software, and shared datasets in electrochemistry and solid state science and technology, by bringing together people from different backgrounds to collaborate.

Hack Week was led by the very capable and engaging team from University of Washington: Dan Schwartz, David Beck, and Matt Murbach. The program kicked off on Monday, May 14 with sessions all day Wednesday through Friday, as well as optional software training tutorials during the week. The activities culminated with project presentations and an optional clamming expedition on Saturday, a traditional activity in the Puget Sound area.

ECS provided hotel room space for both events, and featured Hack Events prominently.

The organizers and participants were delighted with the Hack Week format. It allowed for significant interaction between attendees, and significant training elements. Early tutorials were optional for more experienced software developers.

The schedule for Hack Week was:

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- 0900-1300h (Optional) Social Event (clamming in the Puget Sound area)
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Additionally, the introductory and advanced tutorials throughout the week provided a chance for Hack Week attendees to learn and practice data science and computational skills that were transferable to their own fields/research.

Overall, the success in creating open-software tools, providing educational training, and building an electrochemical data science community was reflected by the responses related to future events:

- 100% of participants in Hack Week would participate in a future ECS Data Science Hack event
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Because data science is a fast moving field, the Showcase will conclude with a “Late Breaking News” session to feature emerging electrochemical and solid state research that embraces open software and open data sets. Especially valued are contributions that feature early-stage research where alpha- and beta-testers can be solicited to improve new open research products. The organizers welcome direct email contact by prospective contributors to the Late Breaking News section, up to four weeks prior to the event.

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M. D. Murbach and D. T. Schwartz (University of Washington)

08:30

DS-2183 (Invited) Tip – Surface Electrode Interactions and the Effects of These Interactions on Scanning Electrochemical Microscopy Response  
A. Mirabal and S. Calabrese Barton (Michigan State University)

09:00

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DS-2184 (Invited) Detailed Chemistry Modeling via Cantera: A Pathway to Understanding Battery Degradation Mechanisms

S. C. DeCaluwe, D. Korff, A. LeBar, A. LeBar (Colorado School of Mines), and C. H. Lee (Colorado School of Mines, University of Colorado, Colorado Springs)

09:30

Break

10:30

DS-2185 (Invited) A Data Science Approach for Quantitative Analysis of Total Differential Capacity Plots

N. L. Thompson, S. Alamdari, T. A. Cohen, R. Masse, G. Cao, V. C. Holmberg, J. Pfaendtner, and D. A. C. Beck (University of Washington)

11:00

DS-2186 (Invited) Using Image Recognition to Identify Platinum Surfaces with Cyclic Voltammetry Scans

H. A. Baroody and T. A. Muzaffar (Department of Chemistry, Simon Fraser University)

11:30

DS-2187 (Invited) Open Science Strategy to Accelerate Adoption of Nonlinear Electrochemical Impedance Spectroscopy as a Battery Diagnostic

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S. Moura (University of California, Berkeley, eCAL), H. Perez, Z. Gima, S. Park, and D. Zhang (University of California, Berkeley)

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Late Breaking News

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**Results Dissemination:** An OSF project page was created to gather the outputs from the ECS Hack Week effort. Each of these projects are more substantial, and have had follow-on work.

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Hendricks, C., Stanley, P., Kononova, O., Haeberle, M., & Saxena, S. (2017, October 4). XPS Data from Li-Ion

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Battery Anodes. Retrieved from [osf.io/58mw9](https://osf.io/58mw9)

Beckner, W. A., Murbach, M. D., & Beck, D. (2017, October 4). Project: Genetic Algorithms with RDKit for Molecular Structure Search. Retrieved from [osf.io/h3zuc](https://osf.io/h3zuc)

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**Honors and Awards:** Nothing to Report

**Protocol Activity Status:**

**Technology Transfer:** All software and datasets associated with Hack Events at ECS are licensed under open access copywriting standards via Creative Commons or MIT licensing. Hack Event research is freely available for reuse by researchers worldwide.

### **PARTICIPANTS:**

**Participant Type:** PD/PI

**Participant:** Daniel Schwartz

**Person Months Worked:** 1.00

Project Contribution:

International Collaboration:

International Travel:

**Funding Support:**

**RPPR Final Report**  
as of 19-May-2020

National Academy Member: N  
Other Collaborators:

**Contract Number:** W911NF1810171

**Title:** ECS Data Sciences Hack Week--Seattle 2018

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Murbach, M. D., Dixit, M., Karuppaiah, C., DeCaluwe, S. C., & Das, T. (2017, October 4). Project: Software tools for analyzing rotating disk electrode data. Retrieved from [osf.io/qrhcw](https://osf.io/qrhcw)

Murbach, M. D. (2017, September 29). Project: Software tools for fitting open-circuit potential data. Retrieved from [osf.io/vebdq](https://osf.io/vebdq)

Hendricks, C., Stanley, P., Kononova, O., Haeberle, M., & Saxena, S. (2017, October 4). XPS Data from Li-Ion Battery Anodes. Retrieved from [osf.io/58mw9](https://osf.io/58mw9)

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Hack Week, Seattle, WA

An OSF project page was created to gather the outputs from the ECS Hack Week effort. Each of these projects are more substantial, and have had follow-on work.

Murbach, M. D., Juhasz, G., Yess, M., Chavan, K., Baroody, H., Teo, L., ... Parke, C. D., 2018 ECS Hack Week Seattle. <https://osf.io/hefmb>

The longer format of the Hack Week provided additional time for deeper project "hacking" focused on:

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Bonezzi, J., Murbach, M. D., Feng, Z., Pang, Q., Dawson-Elli, N., Timbillah, S., & sarfo. (2018, November 29). impedance.py. Retrieved from [osf.io/cpxgj](https://osf.io/cpxgj)

Chavan, K., Budanovic, M., Schwartz, D. T., & Beck, D. (2018, May 17). Redox potential prediction based on molecular properties. Retrieved from [osf.io/x95kw](https://osf.io/x95kw)

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ECS will feature data science in the Spring 2019 Electrochemical Society Interface issue, co-edited by Daniel T. Schwartz, Matthew D. Murbach, and David A.C. Beck, the co-founders of ARO funded ECS Data Science Events. Two papers accepted for publication cite ARO support:

D.T. Schwartz, M.D. Murbach, and D.A.C. Beck, "ECS in the Era of Data Science", ECS Interface, DOI: 10.1149/2.F03191if Accepted (2019).

M.D. Murbach and D.T. Schwartz, "Open Software and Datasets for the Analysis of Electrochemical Impedance Spectra", ECS Interface, DOI: 10.1149/2.F05191if Accepted (2019).

Hack Day and Hack Week data science products are also disseminated as via the Center for Open Science's Open Science Framework (OSF) repository, with individual project component repositories. Research products include the following software and datasets.

## Plans Next Reporting Period

## Honors and Awards

## Protocol Activity Status

## Technology Transfer

All software and datasets associated with Hack Events at ECS are licensed under open access copywriting standards via Creative Commons or MIT licensing. Hack Event research is freely available for reuse by researchers worldwide.

## Distribution Statement:

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Approved for public release; distribution is unlimited.

## Participants

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<b>First Name:</b>	Daniel	<b>Last Name:</b>	Schwartz
<b>Project Role:</b>	PD/PI		
<b>National Academy Member:</b>	N	<b>Months Worked:</b>	1
<b>Countries of Collaboration</b>			