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251st National ACS Meeting

Division of Physical Chemistry

Electrochemistry at Solid/Liquid Interfaces

Oleg Borodin
Yue Qi
Organizers

March 13-15, 2016

San Diego Convention Center

ROOMS 28D & 28C

SUNDAY MORNING * ROOM 28D

Oleg Borodin, Justin Haskins, Presiding

8:00 Introductory Remarks.

8:05 (15). Considering the electrochemical environment in the first-principles modeling of electrocatalytic processes. **A. Gross**, S. Sakong, F. Gossenberger, T. Roman

8:45 (16). Modelling heterogeneous electrocatalysis under realistic conditions. **S.N. Steinmann**, C. Michel, P. Sautet

9:05 (17). Model free method to measure the surface potential of colloidal particles in aqueous solution. C. Luetgebaucks, G. Gonella, **S. Roke**

9:45 (18). Microscopic dynamics of charge separation at the aqueous electrochemical double layer. **A. Willard**, J.A. Kattirtzi, D. Limmer

10:05 INTERMISSION

10:20 (19). Electrochemical reduction, ionization, and solvation of Brønsted acids in ionic liquid solutions. **L. Yu**

10:40 (20). Ultrafast spectroelectrochemistry. S. Toyouchi, Y. Sun, **D.D. Dlott**, N. Garcia Rey

11:00 (21). Potential dependent IR/visible double resonance sum frequency generation spectroscopy to probe electronic structure at electrochemical interfaces. **K. Uosaki**, H. Noguchi, S. Yang

11:20 (22). Nanoscale Li-S battery interfaces investigated with in-situ electrochemical transmission electron microscopy. **K. Jungjohann**, K.L. Harrison, A. Leenheer, N. Hahn, K.R. Zavadil

SUNDAY AFTERNOON * ROOM 28D

Yue Qi and Oleg Borodin, Presiding

1:30 (61). Carbon-electrolyte interfaces and their effect on capacitive energy storage. B. Dyatkin, K. Van Aken, E. Mamontov, N. Osti, H. Wang, J. Black, G. Feng, Y. Zhang, M.K. Thompson, P.T. Cummings, D. Wesolowski, **Y. Gogotsi**

2:10 (62). *Ab initio* simulations of charged interface effects in graphene-based supercapacitors. **B. Wood**

2:50 (63). Dynamic charge storage in nanopores filled with ionic liquids. **R. Qiao**, Y. He, A.A. Kornyshev, J. Huang, B. Sumpter

3:30 INTERMISSION

3:40 (64). Capacitance of graphene-based electrodes from combined first principles and classical simulations. **C. Zhan**, J. Neal, Y. Zhang, J. Wu, P.T. Cummings, D. Jiang

4:00 (65). In-situ study of electric double layers and ionic transport across the solid/liquid interface using scanning probe microscopy. **J. Come**, J. Black, N. Balke

4:20 (66). Modeling charge transfer and dielectric response of atomistic and continuous media. **M.H. Muser**

5:00 (67). Ionic liquids at charged interfaces: Static and dynamic properties from atomistic simulations. **J. Vatamanu**, D. Bedrov

MONDAY MORNING * ROOM 28D

Yue Qi, Presiding

8:00 (109). How SEI forms in aqueous electrolytes. L. Suo, C. Wang, O. Borodin, **K. Xu**

8:40 (110). Mechanism of $Li_xNi_{0.5}Mn_{1.5}O_{4-\delta}$ dissolution in organic carbonate electrolytes. **A. Jarry**, R. Kostecki

9:20 (111). Ab initio molecular dynamics simulations of Mn(II) dissolution from Li(x)Mn(2)O(4) surfaces. **K. Leung**

10:00 INTERMISSION

10:10 (112). Modeling of oxidation decomposition reactions and transition metal dissolution at the electrolyte/cathode interface for the spinel-structured $LiNi_{0.5}Mn_{1.5}O_4$ high-voltage cathode. **M. Olguin**, O. Borodin

10:30 (113). Transport mechanisms in ionic liquid-based electrolytes for magnesium batteries. **G.A. Giffin**, **S. Passerini**

11:10 (114). Roles of solid electrolyte interphases in rechargeable lithium, sulfur and lithium, metal fluoride batteries. **G. Yushin**

MONDAY AFTERNOON * ROOM 28D

Yue Qi, Presiding

1:30 (159). Electrochemical stability of solid electrolytes.**C. Wang**, F. Han

2:10 (160). Electrochemical stiffness in lithium ion battery anodes and cathodes.**A.A. Gewirth**

2:50 (161). Li-doped ionic liquid electrolytes: From bulk phase to interfacial behavior.**J. Haskins**, J. Lawson

3:30 INTERMISSION

3:40 (162). Development of AMOEBA for ionic liquids and applications for Li^+ transport.H. Torabifard, Y. Tu, O.N. Starovoytov, R.E. Duke, **G.A. Cisneros**

4:00 (163). Electrochemical lithiation process into Si substrate. **N. Aoki**, A. Omachi, T. Kondo, K. Uosaki

4:20 (164). Using quartz crystal microbalance with dissipation (QCM-D) measurements to characterize *in situ* Li-ion battery solid-electrolyte interphases. **M.C. Dixon**, Z. Yang, L. Trahey

4:40 (165). Density functional theory screening of gas-treatment strategies for stabilization of high energy-density lithium metal anodes. S. Koch, A. Etxebarria, B. Morgan, O. Bondarchuk, M.Á. Muñoz-Márquez, S. Passerini, **G. Teobaldi**

TUESDAY MORNING * ROOM 28C

Justin Haskins, Presiding

8:00 (208). Improved methods for the *ab Initio* simulation of electrochemical systems. **T.A. Barnes**, D. Prendergast, P. Kent, J. Deslippe, O. Borodin, T.F. Miller

8:40 (209). Understanding the solid electrolyte-electrode interfaces all-solid-state li-ion batteries: First-principles computation on thermodynamics and kinetics. **Y. Mo**

9:20 (210). Structures of THF-solvated sodium ions attracted to a charged molecular surface. **Q. Wu**

9:40 (211). Ultrafast photo-induced electric field at the surfaces of p GaInP2 electrode. **Y. Yang**, M.C. Beard

10:00 (212). Electrochemical characterization of DNA-inspired organic nanowires. **A.G. Wardrip**, A. Mazaheripour, J. Jocson, A. Bartlett, N. Huesken, A. Burke, M.N. Dickson, A.A. Gorodetsky

10:20 (213). Unprecedented efficiency to control orbital energies a vibrational properties of single molecules embedded in electrochemical STM junctions. **I. Baldea**

10:40 INTERMISSION

10:50 (214). Studies of self-exchange electron transfer and charge accumulation at sensitized TiO_2 for multiple-electron-transfer chemistry using a series of amine-functionalized porphyrins. **J. Glancy-Logan**, H. Chen, J.M. Cardon, J. Angsono, S. Ardo

11:10 (215). Light-induced proton conductivity in a photo-acid doped polymer. **S. Haghighat**, S. Ostresh, J. Dawlaty

11:30 (216). Roles of self-exchange electron transfer between anchored metal-polypyridyl dyes to mesoporous metal-oxide thin films. **J. Angsono**, J. Glancy-Logan, H. Chen, S. Ardo