Sang Soo Han, J Nanomed Nanotechnol 2017, 8:6(Suppl)
DOI: 10.4172/2157-7439-C1-057

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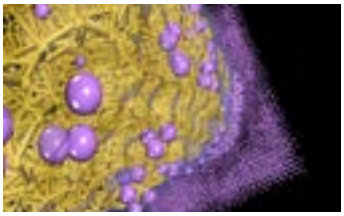
Reactive force field simulation for design of energy-related materials

For the practical use of silicon as anodes for Li-ion batteries, understanding their lithiation and delithiation mechanisms at the atomic level is of critical importance. Also, understanding the nature and formation of the solid-electrolyte interphase (SEI) formed in Li-ion batteries is very significant for improving their functionality. To accurately predict the lithiation/delithiation behaviors of Si anodes and SEI formations between the anode and electrolytes, a computer simulation method to predict chemical reactions in large-scale systems is necessary. In this aspect, a molecular dynamics simulation with first-principles based reactive force fields (ReaxFFs) should be the best choice. In this talk, I will present recent ReaxFF works regarding lithiation/delithiation of pristine, carbon-coated, and oxidized Si nanowires, along with the SEI formation on Si electrodes. And then, I will introduce a multi-scale simulation platform called iBat (battery.vfab.org) for Li-ion battery that has been developed in our research center.



Biography

Sang Soo Han obtained his PhD degree from Korea Advanced Institute of Science and Technology (KAIST), Korea in 2005. From 2005-2009, he was a Post-Doctoral Researcher with Prof. William A Goddard III at California Institute of Technology, USA. Then, from 2009-2013, he worked as a Senior Research Scientist in Korea Research Institute of Standards and Science, Korea. Since June 2013, he has been a Senior/Principal Research Scientist at Korea Institute of Science and Technology, Korea. His research focuses on design of novel energy- and environmental-materials such as battery, catalysis, and gas storage/separation.

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