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Simulation of Bio-Inspired Porous Battery Electrodes

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ABSTRACT

Advancement of technology has led to the increase in use of electronic devices. However, longer life of the rechargeable battery used in electronic devices is one of the biggest issue and demand in the world of electronic devices at present. Battery's performance is affected by the orientation, arrangement, shape and size, and porosity of the materials out of which battery electrodes are made. The goal of this project is to develop a set of numerical libraries that allow developing material micro structures that will allow increasing the performance of rechargeable batteries. We focused on the development of an algorithm that generated porous particle electrodes of controlled particle size and polydispersity. The algorithm intends to develop the simulation tool that captures the randomness and polydispersity of spherical particles, as they occur in real commercial. This application provides very flexible VKML user interface to simulate the generation of particles live. Compared to the existing tools, this application can simulate about 12 times faster for single sized particles and provide a porosity of 56 percent or lower, about 4 times faster for random sized particles to provide the porosity as low as 47 percent or lower, about 2 times faster for 3 different sized particles and provide a porosity of about 43 percent or better, and about 5 times faster for 4 different sized particles to provide porosity as low as 42 percent.

KEYWORDS

Simulation, Battery Electrode, Polydispersity, Porosity, Rechargeable Battery, Electronic Device, VKML

REFERENCES

Chung D.W., Shearing P.R., Brandon N.P., Harris S.J., Garcia R.R., 'Particle Size Polydispersity in Li-Ion Batteries', *Journal of The Electrochemical Society*, *161*(3), A422-A430(2014).

Alex Bartol; R. Edwin García; David R. Ely (2012), "The Virtual Kinetics of Materials Laboratory," https://nanohub.org/resources/vkmllive. (DOI: 10.4231/D34B2X430).