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Systematic and reliable multiscale modelling of lithium batteries[1]

SELCUK ATALAY, [1], MARKUS SCHMUCK, [1] Maxwell Institute and Heriot-Watt University, Edinburgh, UK — Motivated by the increasing interest in lithium batteries as energy storage devices (e.g. cars/bycicles/public transport, social robot companions, mobile phones, and tablets), we investigate three basic cells: (i) a single intercalation host; (ii) a periodic arrangement of intercalation hosts; and (iii) a rigorously upscaled formulation of (ii) as initiated in [1,2,3]. By systematically accounting for Li transport and interfacial reactions in (i)–(iii), we compute the associated chracteristic current-voltage curves and power densities. Finally, we discuss the influence of how the intercalation particles are arranged. Our findings are expected to improve the understanding of how microscopic properties affect the battery behaviour observed on the macroscale and at the same time, the upscaled formulation (iii) serves as an efficient computational tool [4]. [1] M. Schmuck, Appl. Math. Res. eXpr. doi:10.1093/amrx/abx003 (2017). [2] M. Schmuck & M.Z. Bazant, SIAM J. Appl. Math. 75(3):1369-1401 (2015). [3] M. Schmuck & P. Berg, J. Electrochem. Soc. 161(8):E3323-E3327 (2014). [4] A. Ververis & M. Schmuck, J. Comp. Phys. 344:485-498 (2017).

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