

Manuscript Review Report

Title: The influence of crack on the Si anode performance in Na- and Mg-ion batteries: An atomic multiscale study.

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Summary: The study is focused on the effect due to the presence of cracks in the anode on the performance of NIBs and MIBs. Firstly, the authors studied the binding energy for Na and Mg ions in the presence of crack and without it. They found that the binding energies are more in the presence of cracks and the cracks transformed the negative binding energy value in the crack-free surface to a positive value in the presence of a crack. This indicates that cracks provide more energy favourite sites for Na and Mg than those provided by perfect c-Si. After this, the authors studied the Na and Mg diffusion between the crack tip and surrounding regions along the directions of the loading and crack propagation. This analysis uses the migration barrier concept to see if the process is favourable or not and they validated the results through their already calculated binding energy gradient in those regions. They noted that the migration barriers decrease toward the crack tip and the values were found out to be lower than the result of Na diffusion in c-Si. Thus, the crack tip creates a rapid route for Na and Mg to diffuse into the crack. Once they are in the crack, the migration barrier is much more for the ions to diffuse back, therefore the ions tend to diffuse into the crack tip but not in the opposite directions. This may trap interstitials and lower the charging and discharging rate of NIBs and MIBs. Overall, the findings are very interesting.

Minor essential revision: Since figure 4 shows trajectories of Mg diffusion between sites 3 and 1, it would be more precise and readable if it mentioned the same in the figure title.