

Electronic Supplementary Information

A First-Principles Study on Atomic-Scale Pore
Design of Microporous Carbon Electrodes for
Lithium-Ion Batteries†

Young Chul Lee and Sung Chul Jung*

Department of Physics, Pukyong National University, Busan 48513, Republic of Korea

*Corresponding author

Email: scjung@pknu.ac.kr (S. C. Jung)

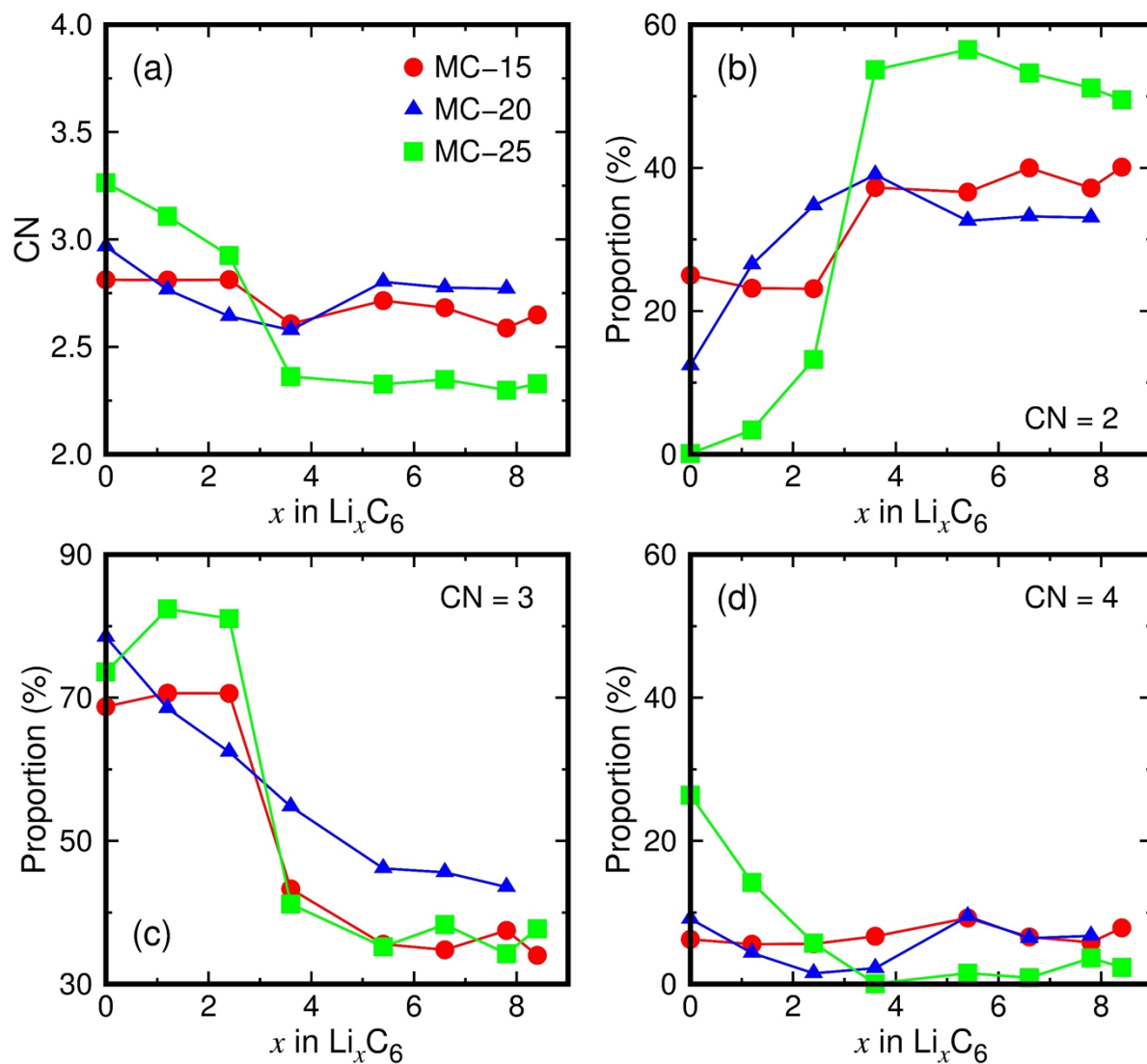


Fig. S1 (a) Average coordination numbers of carbon atoms (CN_{C-C}) and (b–d) proportions of $CN_{C-C} = 2, 3,$ and 4 in lithiated microporous carbon structures with Li atoms removed. $CN_{\alpha-\beta}$ represents the number of β atoms around an α atom. The atomic bond is connected when the C–C distance is within 1.9 \AA .

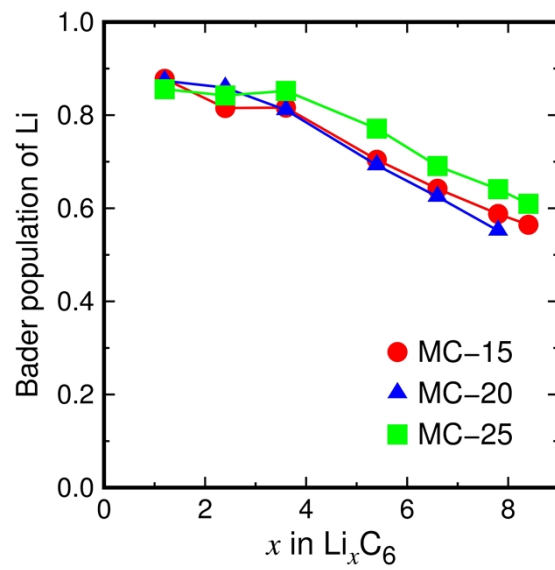


Fig. S2 Average Bader populations of Li in lithiated MC-15, MC-20, and MC-25 structures.

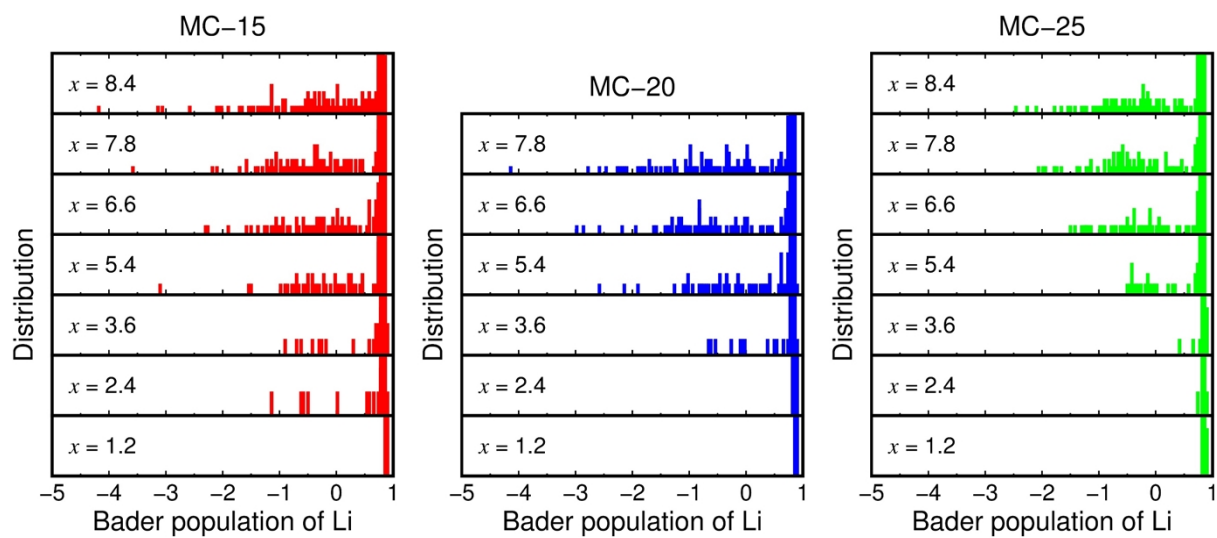


Fig. S3 Distribution histograms of the Bader populations of Li in lithiated MC-15, MC-20, and MC-25 structures.

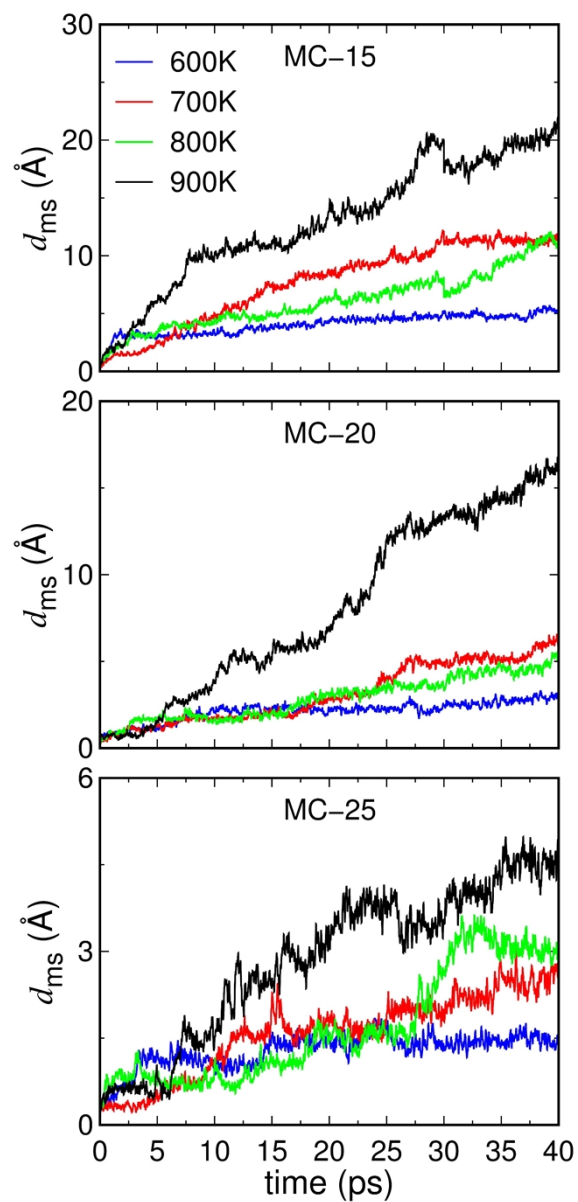


Fig. S4 Mean-square displacements (d_{ms}) of Li atoms in the partially lithiated MC-15, MC-20, and MC-25 ($\text{Li}_{2.4}\text{C}_6$) structures.

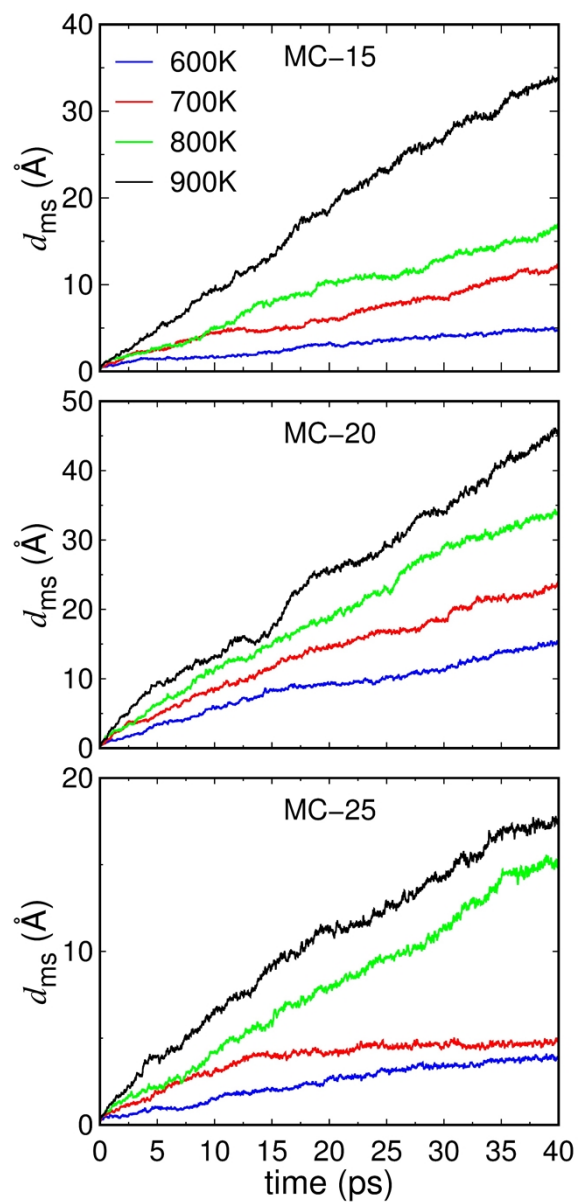


Fig. S5 Mean-square displacements (d_{ms}) of Li atoms in the fully lithiated MC-15 ($\text{Li}_{8.4}\text{C}_6$), MC-20 ($\text{Li}_{7.8}\text{C}_6$), and MC-25 ($\text{Li}_{8.4}\text{C}_6$) structures.