Supporting Information

Kinetic Monte Carlo Study of Ambipolar Lithium-Ion and Electron Polaron Diffusion into Nanostructured TiO_2

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1. Discussion of the limitations of the KMC model

Computational efficiency is an important factor for the applicability of the scale bridging models, such as KMC, to the simulation of complex systems. To estimate the dependence of the computational cost of our KMC model on the particle size we considered the charging process. The time required for a nanoparticle to reach a fully charged state is proportional to the cube of the diffusion coefficient for Li ions. Therefore, the time evolution for the large grains is slower than that of the small grains ($\propto D_{small}^3 / D_{big}^3$), which requires more KMC steps ($\propto D_{big}^3 / D_{small}^3$) during the simulation. Moreover, the computational time for the same charging rate to evaluate each KMC step is also proportional to D_{big}^3 / D_{small}^3. Therefore, the increase in the computational cost for larger grains scales as $\propto D_{big}^6 / D_{small}^6$. This limits the capability of the present method to explore transport properties to grain sizes smaller than 100 nm.

2. Size effect

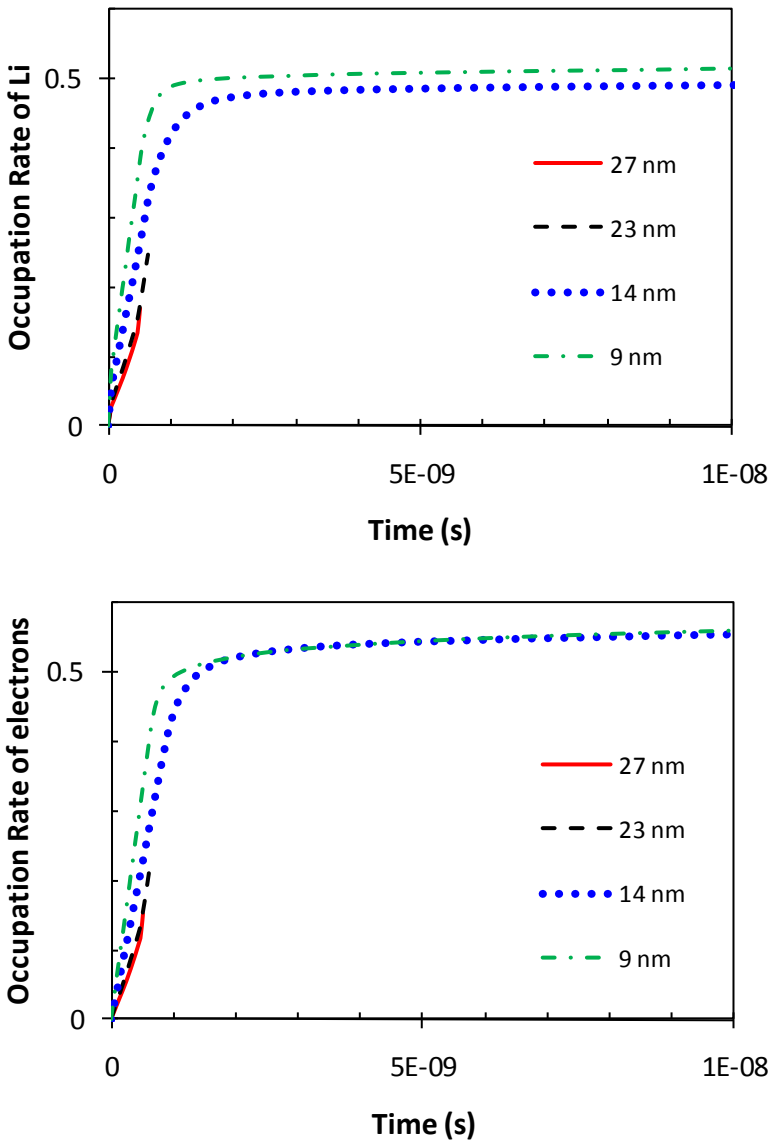

Figure S1. Grain size effect for Li^+ and electron polaron transport in TiO_2 grains with localized carbon coating and sizes 9, 14, 23 and 27 nm. The charge injection rate is $2x10^{10}$ per site per second.