Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Detailed characterization of lithium diffusion mechanisms in crystalline silicon using the kinetic Activation-Relaxation Technique. MICKAL TROCHET, OSCAR ANTONIO RESTREPO GUTIERREZ, NORMAND MOUSSEAU, Universit de Montral — Silicon displays a potential for high-capacity anode material for lithium-ion batteries as it can absorb large quantities of this metal. Yet, very little is understood about the evolution of diffusion mechanisms and migration barriers as the concentration of lithium increases. Until now, for example, simulations studies were limited by the time scale over which diffusion takes place. Here, we use the kinetic activation relaxation technique (kART[1]), an unbiased off-lattice Monte Carlo method with on-the fly catalog building, coupled with the ReaxFF forcefield to follow diffusion of Li in $c-$Si over timescale of seconds and more at room temperature, obtaining detailed information about the whole set of possible diffusion mechanisms as the local environment evolves. We first present a detailed characterization of Li diffusion in the presence of 1 to 3 impurities and then show the evolution of systems with a higher concentration of solute as Li aggregate. These results provide a first detailed picture of the onset of Li aggregating into this high-capacity material, as it modifies the structure through local rearrangements and long-range elastic deformations, crucial information for the development of the next generation of high-capacity anode. \pard\pard[1] M. Trochet *et al*, "Diffusion of point defects in crystalline silicon using the kinetic activation-relaxation technique method," *Phys. Rev. B*, vol. 91, no. 22, p. 224106, 2015.

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Date submitted: 20 Nov 2015 Electronic form version 1.4