Abstract Submitted
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Two orders of magnitude enhancement in Li diffusivity in FCC fullerene under pressure[1] DEYA DAS, AADITYA MANJANATH, Materials Research Centre, Indian Institute of Science, Bangalore, India, SANG SOO HAN, KWANG-RYEOL LEE, Korea Institute of Science and Technology, Seoul 136-791, South Korea, ABHISHEK SINGH, Materials Research Centre, Indian Institute of Science, Bangalore, India — Silicon having high specific capacity of 4200 mAh/g is a potential candidate for anode material in Li ion battery. However, it goes through huge volume change during lithiation and de-lithiation which breaks the electrical contacts. To protect Si anode, carbon based materials have been used experimentally as an artificial solid electrolyte interface (SEI). In order to find a good artificial SEI, Li kinetics also has to be very efficient in it. Here, we theoretically investigated Li kinetics in bulk FCC fullerene and polymerized fullerene modeled by applying hydrostatic pressure. We find that Li diffusion barrier decrease with increasing pressure upto 17.7% volume strain, leading to two orders of magnitude gain in diffusivity compared to the unstrained case. This lowering of barrier can be attributed to the charge transfer triggered by strong interaction between fullerene and Li. Further enhancement of pressure leads to inter-fullerene bond formation that makes Li diffusion barrier high.

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