Abstract Submitted
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Diffusion kinetics and capacity of defected and doped graphene in Li-ion battery[1] RAHUL HARDIKAR, DEYA DAS, Materials Research Center, Indian Institute of Science, Bangalore, India, SEUNGCHUL KIM, SANG SOO HAN, KWANG-RYEOL LEE, Computational Science Center, Korean Institute of Science and Technology, Seoul, South Korea, ABHISHEK SINGH, Materials Research Center, Indian Institute of Science, Bangalore, India — Graphene, with high surface area, electrical conductivity, robust mechanical integrity, has been intensively studied as an anode material for Li ion batteries (LIBs). Better kinetics and reversible storage of Li are desirable characteristics in a LIB. Using first principles calculations, we study the diffusion of Li **through** and **across** the basal plane of defected and doped graphene. The di-vacancy graphene gives the lowest energy barrier of 1.34 eV for Li to diffuse through the layer, while mono-vacancy B doped gives an energy barrier of 0.31 eV for diffusion of Li across the basal plane, indicating across diffusion as the possible mechanism. It is also seen that the capacity of Li storage in doped and un-doped mono-vacancy graphene is several orders greater than its pristine counterparts. Through our study, we show that the defected and doped graphene structures emerge as promising anode materials for application in LIBs.

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Rahul Hardikar
Materials Research Center, Indian Institute of Science, Bangalore, India

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