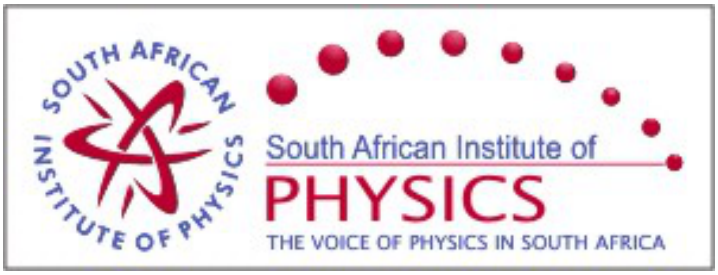

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Ab initio studies of staggered Li adatoms on graphene

We study Li on graphene using the VASP code employing the PAW method within the GGA for the exchange-correlation. We give detailed structural and electronic results for various configurations involving Li on the different two-dimensional unit cells. For 100% coverage, we have new results for Li on the on-top site, which suggests a staggered configuration for the lowest energy structure for which the Li adatoms are alternately pushed into and pulled out of the graphene layer. For 50% coverage, Li favours the hollow site. We have discovered that a careful relaxation of the system also shows a staggered configuration of Lithium adatoms.

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Track Classification: Track A - Condensed Matter Physics and Material Science