Computational modelling of SiC bilayer as anodic material for lithium-ion batteries

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Two-dimensional (2D) materials possess the potential to enhance the capacity and power density of lithium-ion batteries to meet current energy demands. The study of the interaction of lithium with different types of 2D materials is crucial to improving the efficiency of new generations of rechargeable batteries. The size- and geometry-dependent properties in 2D semiconductors, such as 2D silicon carbide and their derived heterostructures, have generated significant interest. 2D SiC. In particular, has shown potential applications in various fields, including high-frequency electronics, photovoltaics, catalysis, and gas sensors [1-3]. In this work we focus on unexplored aspects of the interaction of Li atoms and a 2D SiC bilayer. Li–C, Li–Si and Li–Li interactions and their energetics are studied, making use of analyses of electronic and phonon densities of states, charge density isosurfaces, orbital-projected band structures, and the Crystal Orbital Hamilton Population (COHP). As a result of the vibrational properties of the SiC BL, it was observed that the acoustic modes were restricted with respect to the SiC ML. The computational calculations were performed using the density functional theory, an electronic exchange and correlation potentials were treated with the Perdew-Burke-Ernzerhof functional, within the generalized gradient approximation.

References

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