The influence of intercalation on the surface energy of graphene-like materials

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Using the electron density functional theory, the surface energy of pure and intercalated graphene-like materials [1] is calculated. It is shown that after intercalation by donor-type alkali metal atoms, the surface energy value of graphene-like materials increases. In the case of intercalation by acceptor-type atoms, the surface energy decreases. All calculations were performed using the Quantum Espresso program [2].
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