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First-principles study on interlayer state in alkali and alkaline earth metal atoms intercalated bilayer graphene

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Highlights

- Formation of alkali and alkaline earth metal intercalated bilayer graphene is exothermic reaction except for Be and Mg.
- The interlayer state is occupied for K, Rb, Cs, Ca, Sr, and Ba intercalated bilayer graphene.
- The energetic position of the interlayer state shifts downward monotonically with increasing of the interlayer distance.
- The occurrence of superconductivity is expected for K, Rb, Cs, Sr, and Ba intercalated bilayer graphene whose critical temperature should be smaller than experimentally observed Ca case.

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