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Ab-initio study on stabilized ZnO (0001) polar surface with graphene substrate GUO-HONG CHEN, HONG-JUN XIANG, XIN-GAO GONG, Fudan University — First-principles calculations have been performed on interfaces between zinc oxide (0001) surfaces and graphene layer. By modifying the initial interface configurations we have found the energetically stable interface structure. Results indicate that the unstable polar ZnO (0001) surface could be stabilized by the graphene layer. Further analyses show that the structure stabilization could be well understood by the charge transfer between the carbon atoms and oxygen atoms. This suggests that polar ZnO (0001) surfaces can be obtained in experiments by growing them on graphene substrates.

Guo-hong Chen
Fudan University

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