Hydrogenation of bilayer GaN: Plane orientation and new structures

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In recent years, two-dimensional gallium nitride (GaN) has been theoretically studied and experimentally demonstrated [1]. Unlike other two-dimensional materials such as transition metal dichalcogenides (TMDs), GaN has dangling bonds that are likely to interact with its surroundings, such as a substrate or atoms from the environment. Previous studies have reported that bilayer GaN adopts buckled atomic configurations that differ from that of Xenes and TMDs [2, 3].

In the present work, the impact of hydrogenation on bilayer GaN is studied using first-principles calculations. Our results reveal that the plane orientation of the most stable structure depends on the hydrogen concentration (Figure 1). Unlike in the pristine case, hydrogenated bilayer GaN is not systematically oriented along the c-plane. This plane is the one typically considered in the case of two-dimensional materials. In particular, at high hydrogen concentration, it is shown that the most stable atomic structures are oriented along either the a-plane or the m-plane. First-principles molecular dynamics simulations show that these structures are stable at room temperature. By controlling the temperature and the hydrogen coverage of bilayer GaN, one can therefore control the type of structure obtained, its plane orientation and thus, modulate its properties.

References

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Figures

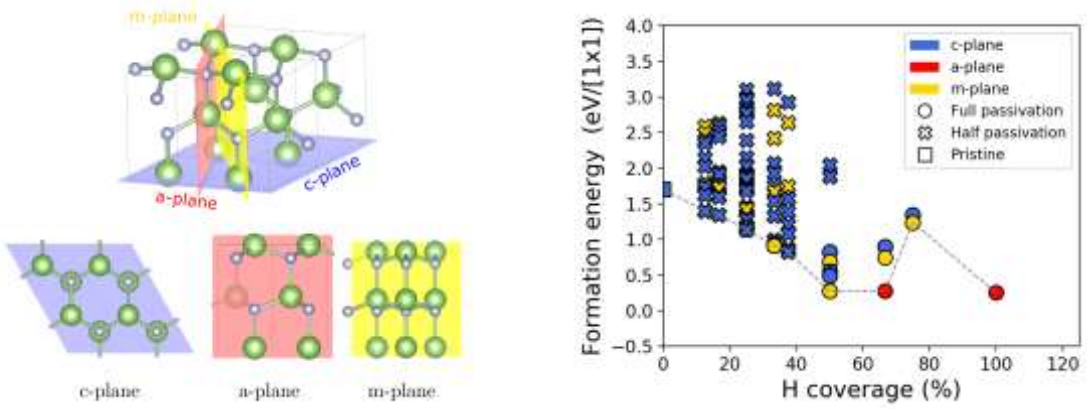

Figure 1: (left) Plane orientations in GaN. Views normal to each plane are shown at the bottom. **(right)** Formation energy with respect to the hydrogen coverage.