Aluminene – 2D allotrope of aluminium

Maja Varga Pajtler[a]
Igor Lukačević[a], Matko Mužević[a], Sanjeev K. Gupta[b]

[a] *Department of Physics, Josip Juraj Strossmayer University of Osijek, Trg Lj- Gaja 6, Osijek 31000, Croatia*
[b]*St. Xavier's College, Department of Physics and Electronics, Ahmedabad 380009, India*

mvarga@fizika.unios.hr

Abstract

After the discovery of graphene, rapid development of experimental methods for syntetization of atomically thin materials took place, as well as theoretical research of other possible ultrathin materials.
Motivated by the huge application potential, inherent from its bulk counterpart, the present study concerns the conditions under which aluminium monolayer, aluminene, could be synthesized in a laboratory for the first time.
In analogy with other monolayer materials, we have employed density functional theory to investigate four different allotropic modifications of aluminium: planar, buckled, triangular and puckered. The study shows that planar and triangular allotropes can be stabilized by strain engineering imposed upon the monolayer and that these allotropes have appropriate cohesive energies and stable lattice dynamics.
We have also verified that Cu(111) and graphene can act as suitable substrates for the synthesis of aluminene, since substrate-monolayer interaction causes the necessary in-plane strain to stabilize the phonon dynamics.
The studied aluminene allotropes are stable with respect to the thermal effects at room temperature and they preserve good thermal properties (specific heat) of aluminium, further advancing its applications as ultra-thin thermal insulator or heatsink.

References

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Figures

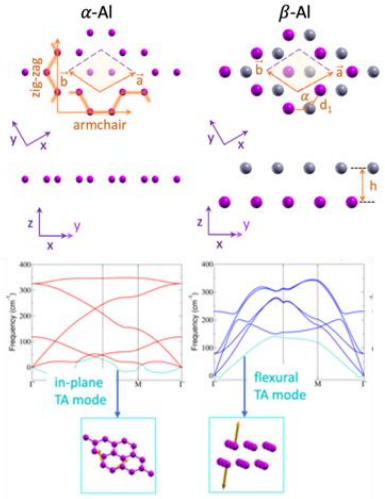

Figure 1: Fully relaxed geometries of planar (left) and buckled (right) allotropes of aluminium and their respective phonon frequencies

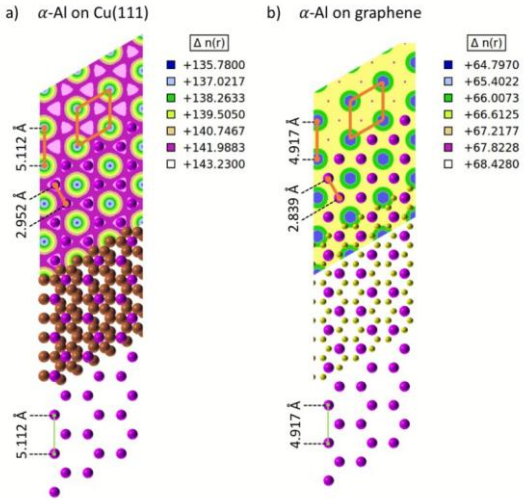

Figure 2: Atomic structure model and STM image of planar aluminene on Cu(111) (a) and graphene (b) superimposed with the adlayer structure