Suitable substrates for the synthesis of stable aluminene allotropes

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Following the example of graphene, recent studies discovered a number of atomically thin monoelemental materials. Many of them were synthesized, while some of them still await their experimental realization [1,2]. Motivated by the huge application potential, inherited from its bulk counterpart, the present study concerns the conditions under which the aluminium monolayer, aluminene, could be synthesized in the laboratory for the first time [3]. We start by considering four different allotropic modifications: planar, buckled, triangular and puckered. The study shows that planar and triangular allotropes can be stabilized by strain engineering imposed upon the monolayer. *Ab initio* simulations show that these allotropes have appropriate cohesive energies and stable lattice dynamics. We discover that Cu(111) and graphene can act as suitable substrates for the synthesis of aluminene. Substrate–monolayer interaction causes the necessary in-plane strain to stabilize the phonon dynamics. The studied aluminene allotropes are stable with respect to thermal effects at room temperature. STM images are simulated to facilitate future experimental characterization of aluminene. Aluminene preserves the good thermal properties (specific heat) of aluminium, further advancing its application as an ultra-thin thermal insulator or heatsink. The study will stimulate experimental studies focused on both nanomaterial synthesis and applications of atomically-thin aluminium layers. At the end further insights into the monolayer-substrate relationship are given.

REFERENCES

[1] G. Li, Y.-Y. Zhang, L. Huang, H. Lu, X. Lin, Y.-L. Wang, Sh. Du, H.-J. Gao, Chem. Soc. Rev., 47 (2018) 6073.
[2] N. R. Glavin, R. Rao, V. Varshney, E. Bianco, A. Apte, A. Roy, E. Ringe, P. M. Ajayan, Adv. Mat., 32 (2020), 1904302.
[3] I. Lukačević, M. Varga Pajtler, M. Mužević, S. K. Gupta, J. Mater. Chem. C, 7 (2019) 2666.

FIGURES

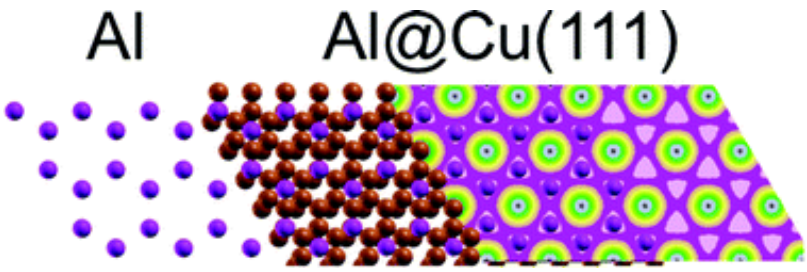

Figure 1: Top-down view of a single-layer aluminene model placed on Cu(111) surface substrate. On the right the predicted STM imaging is shown revealing bright spots where the Al atoms could be found with respect to the bottom Cu atoms.