Properties and feasibility of 2D stacks based on hexagonal AlN sheets

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The intense research dedicated to graphene and its prospective applications motivated and triggered exploration into other two-dimensional (2D) systems. III-Nitride sheets such as 2D hexagonal-BN (h-BN), 2D hexagonal-GaN, and 2D hexagonal-AlN (h-AlN) are among the best candidates to be investigated in the pursuit of prospective graphene alternatives due to the electronic and optoelectronic applications for bulk III-Nitrides [1] on one side, and the structural similarity of their 2D phases to graphene, on the other.
Stability and reactivity issues as well as the electronic properties of 2D III-Nitrides are becoming a focal point of theoretical research. BN monolayers were first predicted theoretically [2] and later experimentally obtained by exfoliation [3].

We predicted the stability of 2D hexagonal-AlN sheets which emerge as a 2D analogue of technologically highly prospective wide-band gap semiconductor Aluminium Nitride.
By performing detailed modelling of the stability of hexagonal AlN (h-AlN) sheets and their structural and electronic properties within the framework of DFT at the GGA-PBE level of theory, we found a lattice parameter of 1.82 Å and an indirect band gap of 2.81 eV as well as a cohesive energy which is by 6% lower than that of the bulk AlN (wurtzite) which is suggestive for the feasibility/synthesizability of individual h-AlN sheets [4].

We also reported on h-AlN typical defects: vacancies, anti-site defects and impurities [4]. Such defects significantly change the band structure in the vicinity of the Fermi level in comparison to the band structure of pristine h-AlN which can be used for deliberately tailoring the electronic properties of h-AlN sheets.

To address functional nanostructures based on h-AlN, we consider different stacking combinations of h-AlN sheets and graphene sheets. The most simple, prototypic h-AlN/graphene stack is illustrated in Fig.1. The structural and electronic properties of more complex stacks depend on the number of h-AlN/graphene sheets and on the stacking configuration [5]. We predict that the integrity of an h-AlN sheet and of 2D stacks based on h-AlN sheets is preserved upon oxidation by oxygen molecules. This is another indication for the feasibility of h-AlN-based stacks and even corresponding layered systems [5]

If synthesizable, the layered materials based on stacked hexagonal AlN sheets may play an essential role as substrates for growth of integrated nanostructures for optoelectronic applications, including LEDs and solar cells. They also may be prospective templates for novel hydrogen storage materials.

In this presentation we'll emphasize our encouraging theoretical findings on h-AlN in the context of the vast competence and experience on growth of III-Nitrides available in our group at Linköping University in Sweden [6, 7].

References
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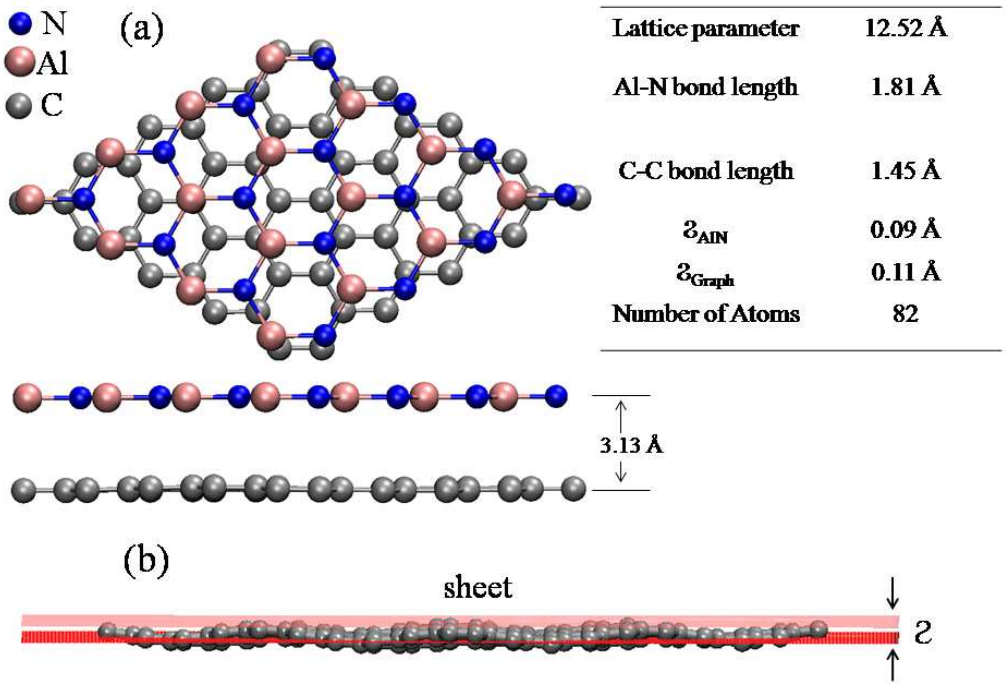

Figure 1: (a) The most simple stacked system consisting of one h-AlN and one graphene sheet. Structural features such as lattice parameters as influenced by the stacking and bond lengths as well as the inter-sheet equilibrium distance are also shown. (b) The buckling resulting from the relaxation of the stacking configuration consists in smooth 2D ripples. This buckling can be described by the perpendicular atomic displacement z.