

# Planar versus three-dimensional growth of metal nanostructures at graphene

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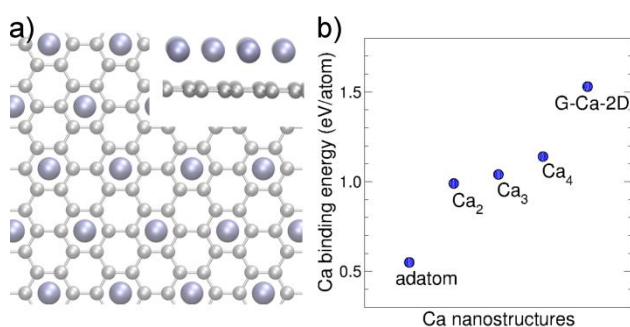
Atomic scale description of graphene (G) contacts with metals is of critical importance for development of efficient G-based nanoelectronic devices. Depending on the growth mode of metals on G they can form smooth ultra-thin films or three-dimensional (3D) nanostructures with markedly different electrical contacts. Employing density functional theory we studied microscopic mechanisms governing initial stages of growth of three selected metals (Li, Ti and Ca) on G. Tendency towards planar or 3D growth is rationalized based on description of the interaction between metal adatoms, as well as adsorption geometries of their trimers and tetramers. Li atoms, featuring a long-ranged electro-static repulsion, are individually dispersed across the surface, in a sharp contrast with atoms of transition metal Ti which gather into densely-packed 3D clusters due to a strong short-ranged metal-metal attraction. Modest attractive interaction between Ca adsorbates enable formation of mono-atomic films with the local coverage of 1/6 monolayer – structure with great stability and high density of states at Fermi level. Since Ca adsorbates induce nearly three-fold increase in adhesion energy between G layers, Ca intercalated carbon sheet falls into category of functionalized materials with promising properties for engineering

high quality contacts in vertical heterostructures of 2D materials.

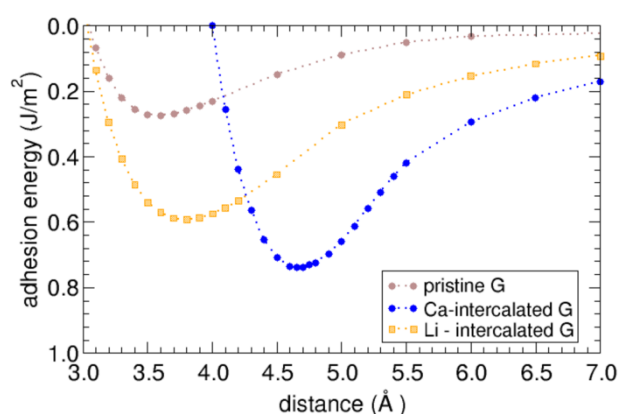
## References

- [1] S. Stavić, M. Belić, Ž. Šljivančanin, Carbon 96 (2016) 216-222

## Figures



**Figure 1:** a) The most stable 2D nanostructure of Ca at graphene (G-Ca-2D); b) Trends in Ca binding energy as a function of the size of Ca nanostructures.



**Figure 2:** Bilayer graphene - adhesion energy as a function of distance between graphene layers for pristine, Ca-intercalated and Li-intercalated graphene bilayers. The calculation are performed applying optB88-vdW functional.