

Graphene derivatives: CVD Growth, characterization and modelling

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The CVD growth of graphene on metal foils from precursors other than methane offers several advantages. While using ethanol vapours and lowering the growth temperature, the growth of electrically insulating and optically transparent films is observed down to temperatures as low as 500°C.

However the catalytic growth of carbons beyond the fully sp² and ultra-stable graphene, requires the careful planning of the entire growth process and post-growth processing. Several diagnostics must be carefully applied for the correct assessment of the evanescent properties of functionalized atomic layers.

We investigated by first principles calculations the thermodynamic stability of functionalized graphene derivatives, and predicted optical, electronic and magnetic properties for some of them.