## CHEM2DMAC

## Carbide Formation at Graphene/Nickel Interface: The Decisive Role of Graphene Orientation

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When graphene (G) is grown on nickel substrate, the restructuring of the metallic surface upon carbon segregation resulted in the formation of nickel carbide (Ni<sub>2</sub>C) phase at the interface but solely in rotated graphene (RG) domains and not under the epitaxial graphene (EG) [1]. Motivated by this experimental puzzle, we perform density functional theory calculations to illuminate the microscopic mechanisms governing the structural changes of a C-rich nickel surface under G cover [2]. We show that high concentration of subsurface carbon destabilizes the Ni(111) surface and gives rise to the formation of thermodynamically advantageous Ni<sub>2</sub>C monolayer. We point out the crucial role of G rotation in enabling high density of favorable C binding sites in nickel subsurface. As opposed to RG, EG cover locks the majority of favorable C binding sites preventing the build-up of subsurface carbon density to a phase transition threshold. In line with strong experimental evidence, we explain why the Ni<sub>2</sub>C phase formation can take place only if G is misaligned with the Ni(111) surface.

## References

- [1] C. Africh, C. Cepek, L. Patera, et al., Sci. Rep. 6, 19734 (2016).
- [2] S. Stavrić, S. Del Puppo, Ž. Šljivančanin, M. Peressi, Phys. Rev. Materials 5, 014003 (2021).

## **Figures**



Figure 1: dependence of binding energy of subsurface carbon on the concentration of C atoms at RG/Ni(111) (red) and EG/Ni(111) (blue) interfaces.