

# ***N*-Heterocyclic Carbenes as Modifiers of Metal-Supported Graphene**

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## Abstract

*N*-heterocyclic carbenes (NHCs) provide a new method to functionalize graphene. We have demonstrated the NHC functionalization of graphene monolayers on Pt(111) and Ru(0001)[1]. As probed using reflectance IR spectroscopy, the grafted NHCs display thermal stabilities similar to that reported for aryl groups on graphite and graphene. Differences in the strength of the interaction between the Gr/Pt(111) and Gr/Ru(0001) systems are attributed to their respective p-doped and n-doped characters coupled with the electron-donor property of the NHC. Intercalation of oxygen between graphene and Ru(0001) leads to NHC bonding similar to that for Gr/Pt(111) consistent with the removal of the strong Gr/Ru interaction to form a quasi-freestanding p-doped layer. These observations are significant since NHCs form an extremely diverse family of compounds that may enable custom approaches to modify graphene for specific applications. The persistent character intrinsic to NHCs should facilitate functionalization from the vapor-phase while limiting co-deposition of dimerization products. For the same reason, NHCs may offer greater homogeneity of functionalization in that they are less indiscriminately reactive than aryl radicals or simple carbenes. Observations related to catalysis will be discussed.

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## References

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- [1] T. Zhang, S. B. Khomane, I. Singh, C. M. Crudden, P. H. McBreen, *J. Phys. Chem. C* 126 (2022) 14430.