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# Molecular Junctions between Graphene Nanoplatelets to Enhance Heat Transfer in Nanomaterials

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The fast-growing development of modern technologies made efficient heat dissipation extremely important to the performance, lifetime and reliability of electronic and optoelectronic devices. In this context, freestanding graphene nanopapers have emerged as promising materials to address heat dissipation problems in practical applications.[1] However, the thermal conductivity of such networks is strongly limited by the inefficiency of the contacts between graphene sheets.

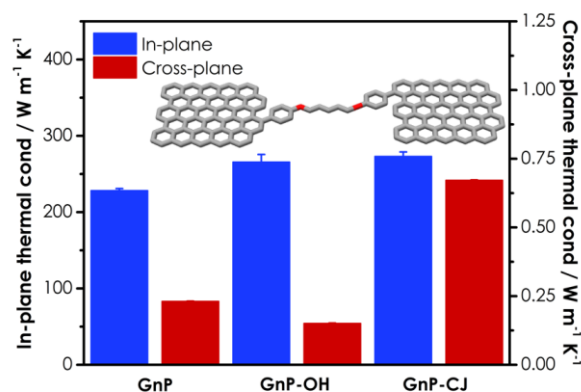
The aim of this study is to design and synthesize molecular junctions between graphene nanoplatelets (GnP) to create graphene nanopapers with inherently low contact thermal resistance among nanoparticles. Molecular dynamics was used to screen for candidate molecules to enhance conductance at the particle-particle contacts, including chain length and bonding method. Covalent and non-covalent synthetic approaches were exploited to engineer contact resistance in graphene networks. Covalent functionalization was recently demonstrated to enhance both in-plane and cross-plane thermal conductivity of GNP networks. (Figure 1).[2] Non-covalent functionalization, by the use of bispyrene derivatives to build supramolecular junctions between nanoplatelets, was also observed to strongly influence the heat transfer on the network,

also depending on the chain length of the alkyl spacer between pyrene groups (Figure 2).

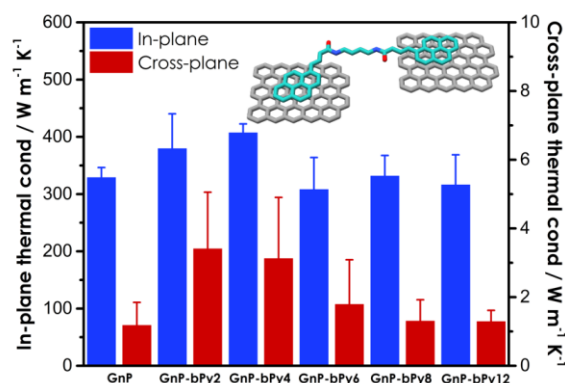
## References

- [1] Balandin, A.A., Nat. Mater, 10 (2011) 569
- [2] Bernal, M.M.; Di Pierro, A.; Novara, C.; Giorgis, F.; Mortazavi, B.; Saracco, G.; Fina, A., Adv. Funct. Mat., (2018) 1706954

## Figures



**Figure 1:** In-plane and cross-plane thermal conductivities of GnP and functionalized GNP with supramolecular and covalent junctions.



**Figure 2:** In-plane and cross-plane thermal conductivities of GnP and functionalized GNP with bispyrene derivatives (GnP-bPyx).