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Line defects in Graphene: How doping cures the electronic and mechanical properties DANIEL BERGER, CHRISTIAN RATSCH, Department of Mathematics, UCLA — Graphene and carbon nanotubes have extraordinary mechanical properties. Intrinsic line defects such as local non-hexagonal reconstructions or grain boundaries, however, significantly reduce the tensile strength and destroy its unique electronic properties. Here, we address the properties of line defects in graphene from first-principles on the level of full-potential density functional theory, and assess doping as one strategy to strengthen such materials. We carefully disentangle the global and local effect of doping by comparing results from the virtual crystal approximation with those from local substitution of chemical species, in order to gain a detailed understanding of the breaking and stabilization mechanisms. We find that n-type doping or local substitution with electron rich species increases the ultimate tensile strength significantly. In particular, it can stabilize the defects beyond the ultimate tensile strength of the pristine material. We therefore propose that this should be a key strategy to strengthen graphenic materials. We find that doping can furthermore lead to semi-conducting behaviour along line defects, ultimately restoring the unique electronic properties of graphene.

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