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Computational Design of Graphene Nanoscrolls. KARTEEK BEJAGAM, Virginia Tech , SAMRENDRA SINGH, Scientist, SANKET DESHMUKH, Assistant Professor, DESHMUKH GROUP TEAM, SAMRENDRA GROUP COLLABORATION — Graphene nanoscrolls have obtained a significant interest in recent years due to their potential applications in tribology, nanotechnology, and bioengineering. For example, recently it has been shown that graphene nanoscrolls can be used to experience superlubricity – almost zero friction state. In the present study we employ the metal/non-metal nanoparticles to facilitate the graphene nanoscroll formation. We have conducted reactive molecular dynamics (RMD) simulations of diamond, Nickel, and Gold nanoparticles placed on the 2D graphene sheet. RMD simulations reveal the mechanisms that facilitates or prohibits the graphene nanoscroll formation. Our simulations suggest that the surface chemistry and interactions between nanoparticles and graphene play a crucial in determining the mechanism of scroll formation and the nature of the nanoscroll. We also find that the type of a nanoparticle has strong influence on the elastic and mechanical properties of the nanoscroll. Our study provides a systematic pathway to design graphene nanoscrolls with a wide range of properties.

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