

Abstract Submitted
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Controllable defect healing and N-doping of graphene by CO and NO molecules¹ BIN WANG, Department of Physics and Astronomy, Vanderbilt University, SOKRATES PANTELIDES, Department of Physics and Astronomy, Vanderbilt University and Oak Ridge National Laboratory — Controllable defect healing and N-doping in graphene would be very valuable for potential device applications. Here we report first-principles molecular dynamic simulations that suggest a procedure with fast dynamics and low thermal budget. Vacancies can be healed by sequential exposure to CO and NO molecules. A CO molecule gets adsorbed at a vacancy site and a NO molecule subsequently removes the extra O by forming NO₂. Controllable N-doping can be achieved by sequential vacancy creation (e.g. by electron beam) and subsequent exposure to NO molecules at room temperature. A combination of CO and NO molecules can potentially provide simultaneous healing and doping at a desirable ratio. The proposed strategy introduces no extra defects and is promising for graphene-based materials in radiation environments.

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